Exceptional service in the national interest

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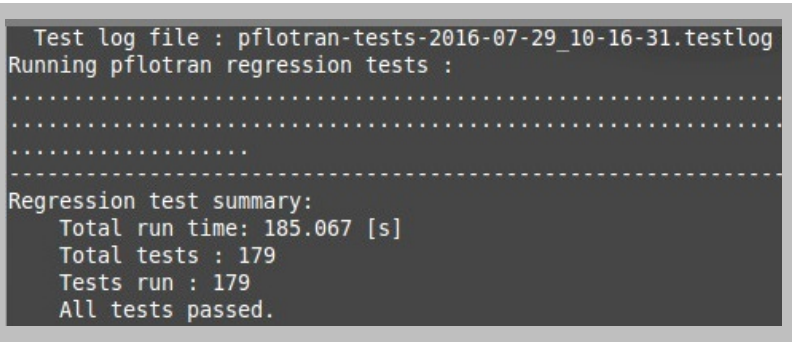

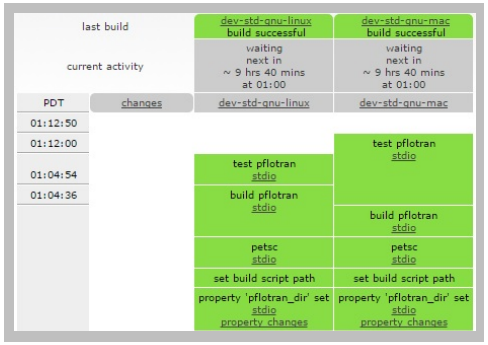

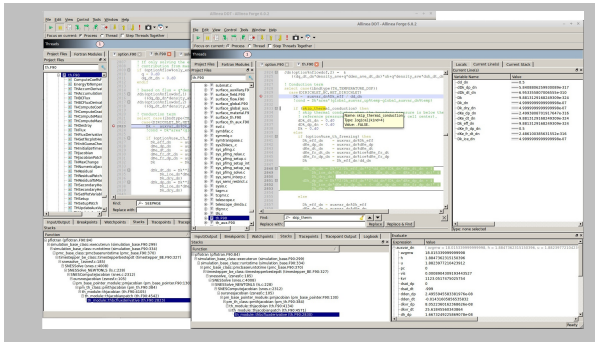

Putting It All Together: Example

PFLOTRAN

Glenn Hammond

August 8, 2016

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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Outline

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- Introduction to PFLOTRAN
- Code development
  - IDEs
  - Refactoring
  - Testing
  - Debugging
- Open source deployment
  - Software repository
  - Documentation
  - User support
  - QA

PFLOTRAN

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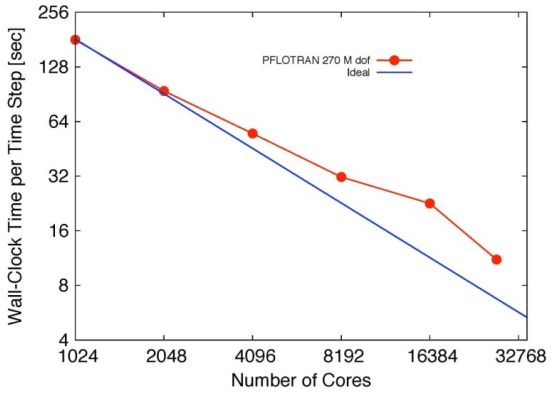
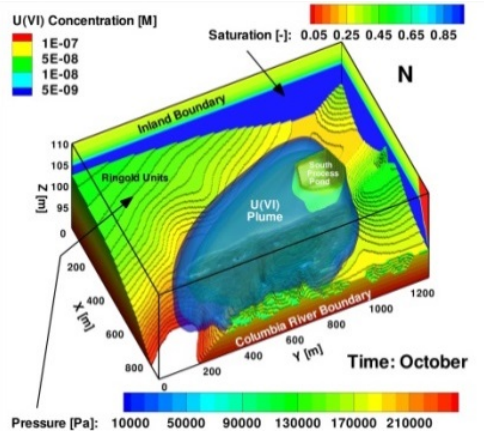
- Petascale reactive multiphase flow and transport code
- Open source license (GNU LGPL 2.0)
- Object-oriented Fortran 2003/2008
  - Pointers to procedures
  - Classes (extendable derived types with member procedures)



- 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

Numerical Methods

- Spatial discretization
  - Finite volume (2-point flux default)
  - Structured and unstructured grids
- Time discretization: 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

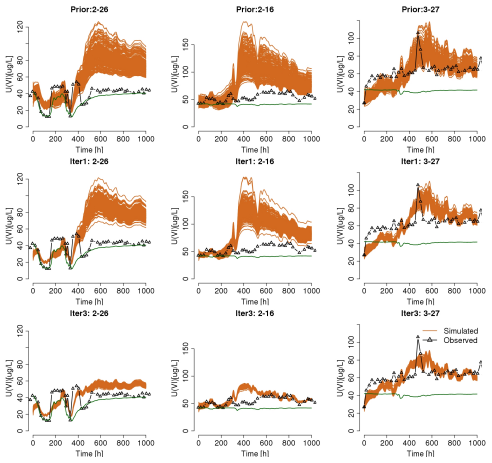
Deep Borehole Waste Disposal

Emily Stein, SNL, 2015

PFLOTRAN Computing Capability

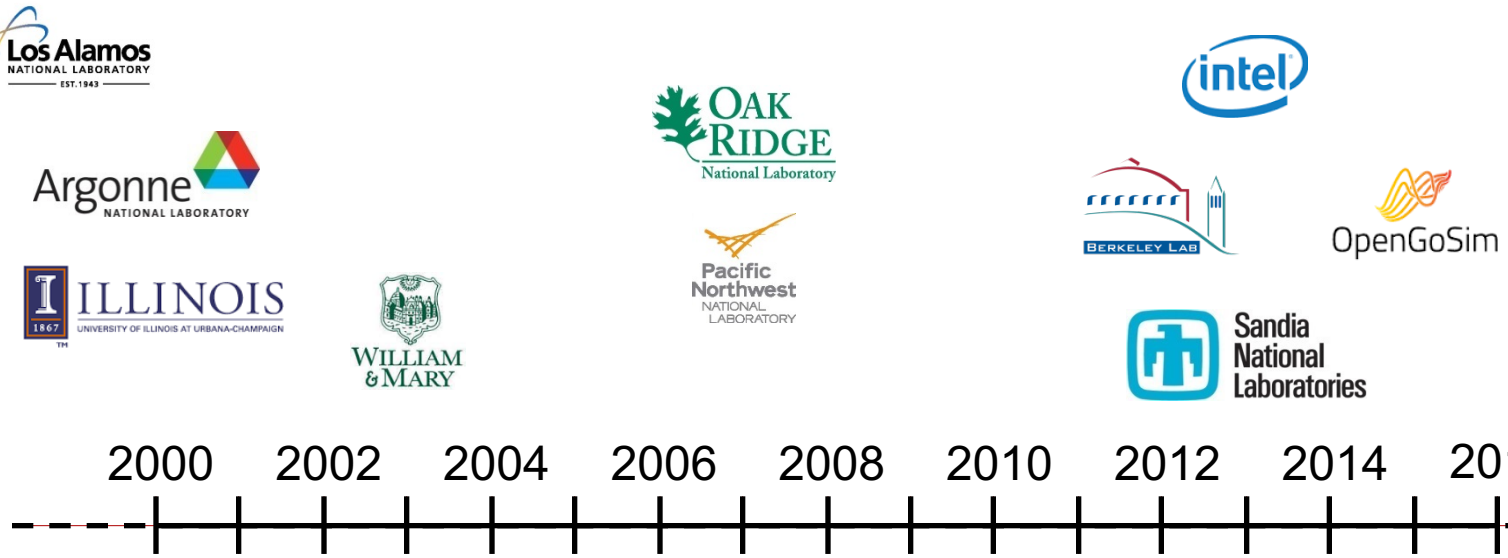
- High-Performance Computing (HPC)
  - Increasingly mechanistic process models
  - Highly-refined 3D discretizations
  - Massive probabilistic runs
- Open Source Collaboration
  - Leverages a diverse scientific community
  - Sharing among subject matter experts and stakeholders from labs/universities
- 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

PFLOTRAN Development Timeline



PFLOTRAN Developers

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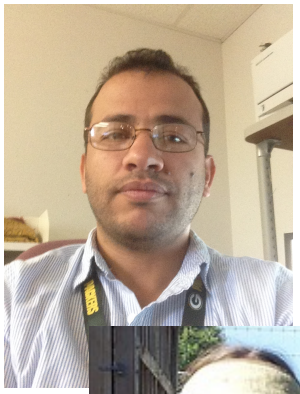





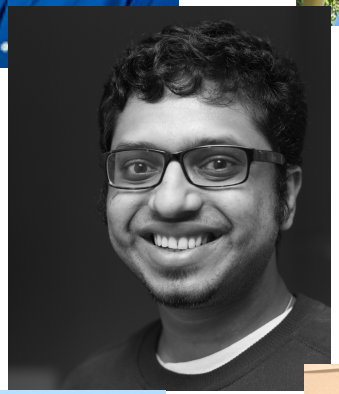

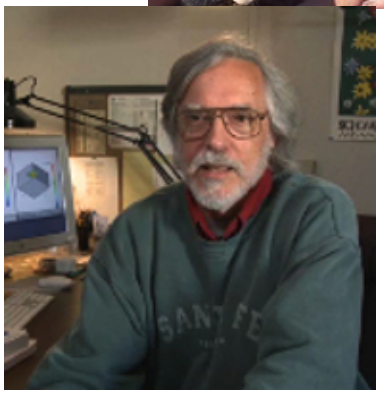


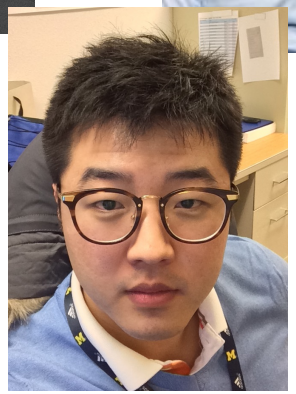

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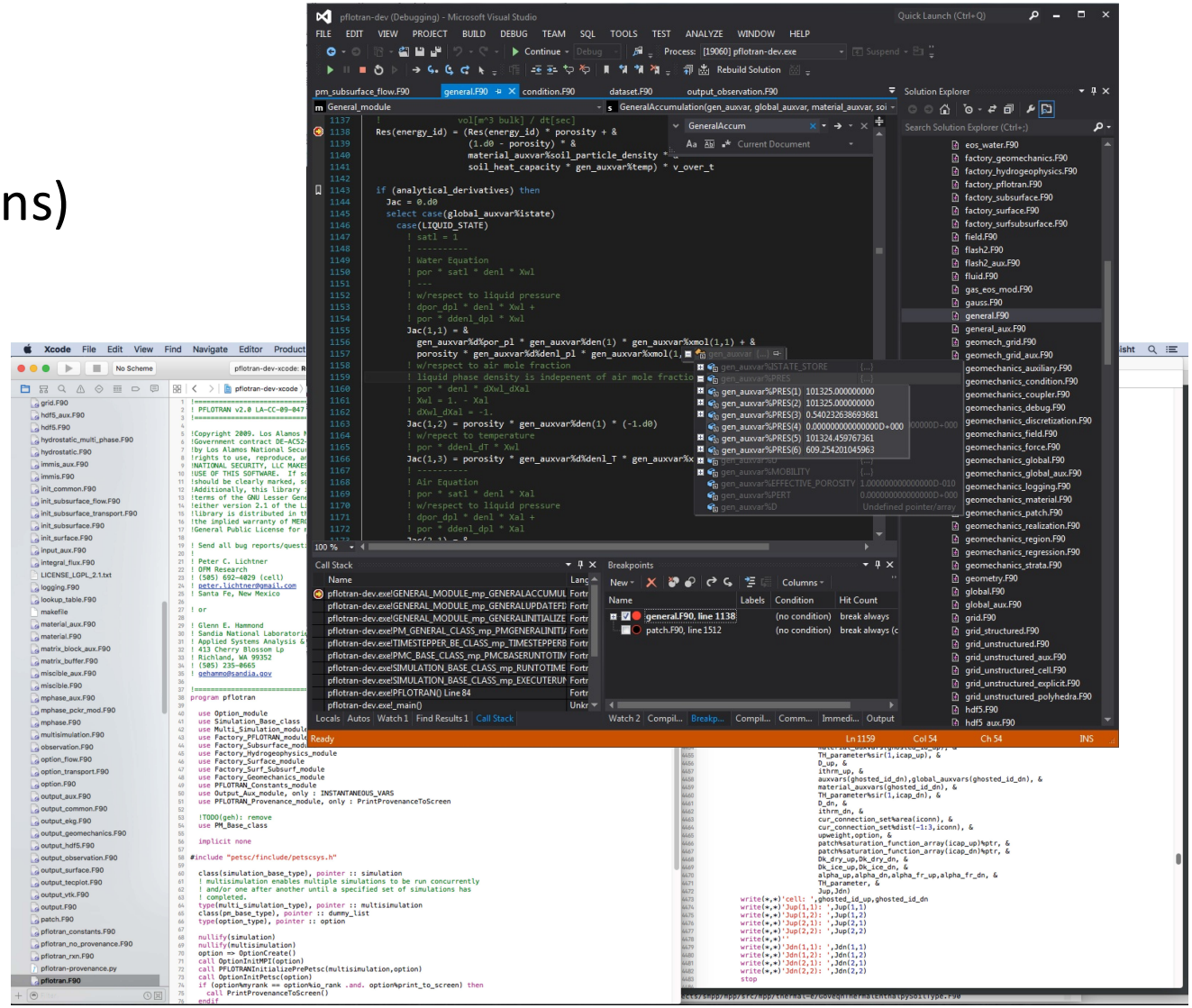
CODE DEVELOPMENT

IDEs

- Emacs
- gVim (w/plugins)
- Kate
- Visual Studio
- Xcode

Bottom line: Pick one that best suites your development style.



Benefits of IDEs during Development and Refactoring

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- Automated generation of dependency lists
- Bookmarks
- Code completion
- Formatting (auto-indent, block indent, etc.)
- Global search and replace
- Syntax coloring/highlighting and checking
- Integrated compiler
  - Linkage of compile-time errors to lines in source
- Integrated debugger

Testing

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- Unit testing
  - Equations of state
    - Viscosity
    - Density
    - Enthalpy / internal energy
    - Saturation pressure
  - Constitutive relations
    - Capillary pressure functions
    - Saturation functions
    - Relative permeability functions
  - pFUnit
    - Open source Fortran unit testing framework

Testing (cont.)

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- Regression testing (Did the solution change?)
  - Driven by custom python scripting
  - Regression module in PFLOTRAN used to sample solution variables at the end of a simulation
  - Locations (cell ids) are specified in a REGRESSION block

```
REGRESSION
  CELLS_PER_PROCESS 2
  CELLS
    29
/
END
```

  - Variables are specified in the OUTPUT block
  - `.regression` file compared to `.regression.gold` file
  - Solutions outside absolute- or relative-change convergence tolerances are flagged.

Regression Entries in Input File

```
#========================== regression =====================================
REGRESSION
  CELLS_PER_PROCESS 2
  CELLS
    29
  /
END

#========================== output options ==================================
OUTPUT
  VARIABLES
    LIQUID_PRESSURE
    LIQUID_SATURATION
    PERMEABILITY_X
    PERMEABILITY_Y
    PERMEABILITY_Z
    POROSITY
    PH
    TOTAL
    TOTAL_SORBED
    KD
    MINERAL_SATURATION_INDEX
  /
END
```

.regression Output File

```
-- PRESSURE: Liquid Pressure --
      Max:   3.6987012374958E+05
      Min:  -2.9546226998033E+04
     Mean:   1.7789073395768E+05
       29:   1.9047483535024E+05
        1:   3.6938752319775E+05
       31:   1.9834550275718E+05
-- RATE: Metatorbernite Rate --
      Max:   0.0000000000000E+00
      Min:  -1.9999999998411E-11
     Mean:  -2.6666666663803E-12
       29:   0.0000000000000E+00
        1:   0.0000000000000E+00
       31:   0.0000000000000E+00
-- GENERIC: LIQUID VELOCITY [m/d] --
       29:   8.5124089175370E-02 -1.2877090842582E-01  5.2164253201197E-04
        1:   1.7617702348986E-02 -9.6502560583815E-04 -8.0086946328361E-04
       31:   2.5578704112122E-01  2.2363909790982E-02  1.8169543176494E-02
-- SOLUTION: Flow --
   Time (seconds):   2.6570320129395E-02
   Time Steps:           14
   Newton Iterations:           28
   Solver Iterations:           28
   Time Step Cuts:            0
   Solution 2-Norm:   1.8527721282346E+06
   Residual 2-Norm:   3.7495263161587E-13
```

Testing (cont.)

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- Tests can be launched through the PFLOTRAN makefile
  - `make rtest` (regression tests only)
  - `make utest` (unit tests only)
  - `make test` (regression and unit tests)

- Regression tests can be launched separately from the command line within `$PFLOTRAN_DIR/regression_tests`

```
python regression_tests.py <args>
```

python regression_tests.py --help

```
usage: regression_tests.py [-h] [--backtrace] [--advanced]
                           [-c CONFIG_FILES [CONFIG_FILES ...]] [--check-only]
                           [--check-performance] [--debug] [-d]
                           [-e EXECUTABLE] [--list-suites] [--list-tests]
                           [-m MPIEXEC] [-n]
                           [-r [RECURSIVE_SEARCH [RECURSIVE_SEARCH ...]]]
                           [-s SUITES [SUITES ...]] [-t TESTS [TESTS ...]]
                           [--timeout TIMEOUT] [-u]

Run a pflotran regression tests or suite of tests.

optional arguments:
  -h, --help            show this help message and exit
  --backtrace           show exception backtraces as extra debugging output
  --advanced            enable advanced options for developers
  -c CONFIG_FILES [CONFIG_FILES ...], --config-files CONFIG_FILES [CONFIG_FILES ...]
                        test configuration file to use
  --check-only          diff the existing regression files without running
                        pflotran again.
  --check-performance   include the performance metrics ('SOLUTION' blocks) in
                        regression checks.
  --debug               extra debugging output
  -d, --dry-run         perform a dry run, setup the test commands but don't
                        run them
  -e EXECUTABLE, --executable EXECUTABLE
                        path to executable to use for testing
  --list-suites         print the list of test suites from the config file and
                        exit
  ...
```

543.cfg – Regression Test Configuration File

```
[suites]
standard = 543_flow
           543_flow_dbase
           543_flow_eos_default
           543_flow_eos_constant
           543_flow_eos_exponential
           543_flow_and_tracer
           543_flow_and_tracer_dbase
           543_hanford_srfcplx_base
           543_hanford_srfcplx_base_restart
           543_hanford_srfcplx_base_restart_hdf5
           543_hanford_overwrite_restart
           543_hanford_srfcplx_param
standard_parallel = 543_flow-np8
                    543_flow_and_tracer-np8
                    543_hanford_srfcplx_param-np8

[default-test-criteria]
# default criteria for all tests, can be overwritten by specific tests
time = 500 percent
generic = 1.0e-12 absolute
concentration = 1.0e-9 relative
discrete = 0 absolute
rate = 1.0e-12 absolute
volume_fraction = 1.0e-12 absolute
pressure = 1.0e-12 relative
saturation = 1.0e-12 absolute

...

[543_flow-np8]
np=8

[543_hanford_srfcplx_param]
generic = 1.0e-12 relative
```

make test Screen Output

```
[fuji]pflotran-dev/src/pflotran(110): make test
make[1]: Entering directory `/home/gehammo/software/pflotran-dev/src/pflotran/un
ittests'
------------------------------------------------------------------------
Running pflotran unit tests :
....................................
Time:         0.001 seconds

 OK
 (38 tests)
------------------------------------------------------------------------
make[1]: Leaving directory `/home/gehammo/software/pflotran-dev/src/pflotran/uni
ttests'
make[1]: Entering directory `/home/gehammo/software/pflotran-dev/regression_test
s'
/usr/bin/python regression_tests.py -e ../src/pflotran/pflotran  --mpiexec /home
/gehammo/local/bin/mpiexec \
                --suite standard standard_parallel \
                --config-files ascem/batch/batch.cfg ascem/1d/1d-calcite/1d-calc
```

```
  Test log file : pflotran-tests-2016-07-29_10-16-31.testlog
Running pflotran regression tests :
........................................................................
........................................................................
...................
------------------------------------------------------------------------
Regression test summary:
    Total run time: 185.067 [s]
    Total tests : 179
    Tests run : 179
    All tests passed.
```

Testing (cont.)

- Example regression 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
```

```
------------------------------------------------------------------------
Running pflotran unit tests :
...F.....................................
Time:         0.001 seconds

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

 FAILURES!!!
Tests run: 38, Failures: 1, Errors: 0
------------------------------------------------------------------------
make[1]: Leaving directory `/home/gehammo/software/pflotran-dev/src/pflotran/uni
ttests'
make[1]: Entering directory `/home/gehammo/software/pflotran-dev/regression_test
s'
/usr/bin/python regression_tests.py -e ../src/pflotran/pflotran  --mpiexec /home
/gehammo/local/bin/mpiexec \
                --suite standard standard_parallel \
                --config-files ascem/batch/batch.cfg ascem/1d/1d-calcite/1d-calc
```

```
  Test log file : pflotran-tests-2016-07-29_10-27-50.testlog
Running pflotran regression tests :
............F.F....FFFFF..F..F.....F...........F..FFFF.FFFF......F.....F...FFFF.
...FF.................F.F...FF.F.................F..F.............FF.............
....F..............
------------------------------------------------------------------------
Regression test summary:
    Total run time: 178.551 [s]
    Total tests : 179
    Tests run : 179
    Failed : 37
```

pflotran-tests-2016-07-29_10-27-50.testlog

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```
PFLOTRAN Regression Test Log
Date : 2016-07-29_10-27-50
System Info :
    platform : linux2
Test directory :
    /home/gehammo/software/pflotran-dev/regression_tests

PFLOTRAN repository status :
---------------------------
$ hg parent
changeset:   10149:f9f01bbf557a
tag:         tip
user:        Glenn Hammond
date:        Thu Jul 28 18:59:00 2016 -0700
summary:     Modified seepage face BC in TH to prevent thermal conduction when boundary pressure is below the
reference pressure (e.g. river stage below cell center).

$ hg status -q
M src/pflotran/eos_water.F90

PETSc information :
-------------------
* WARNING * This information may be incorrect if you have more than one
    version of petsc installed.
    PETSC_DIR : /home/gehammo/software/lib/petsc-git
    PETSC_ARCH : gnu-c-debug
    petsc repository status :
$ git log -1 HEAD
commit 9fc87aa74b00c10f6fbaa6e6828460251b027710
Author: Barry Smith <bsmith@mcs.anl.gov>
Date:   Mon Jun 6 15:16:46 2016 -0500

    Add additional information to MATSOLVERMUMPS manual page
```

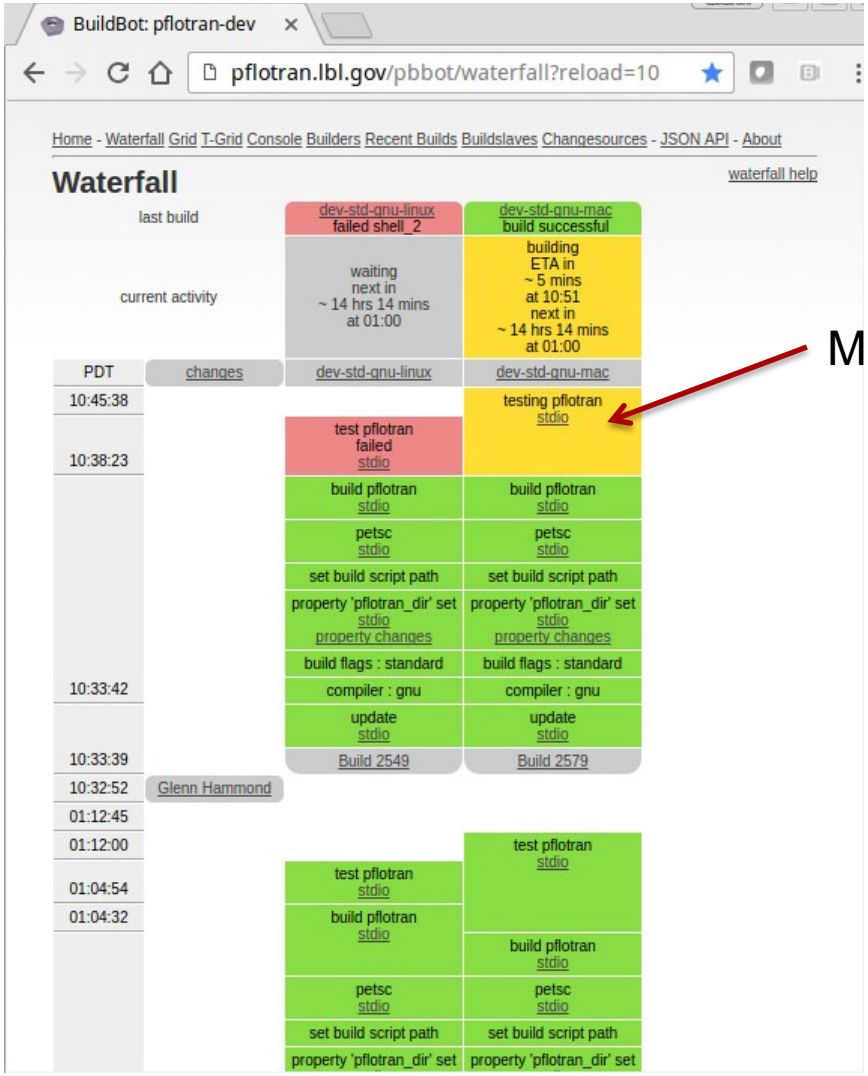
pflotran-tests-2016-07-29_10-27-50.testlog

```
---------------------------------------
543_flow-np8...
    cd /home/gehammo/software/pflotran-dev/regression_tests/default/543
    /home/gehammo/local/bin/mpiexec -np 8 /home/gehammo/software/pflotran-dev/src/pflotran/pflotran -malloc 0 -
successful_exit_code 86 -input_prefix 543_flow-np8
    # 543_flow-np8 : run time : 1.31 seconds
    diff 543_flow-np8.regression.gold 543_flow-np8.regression
543_flow-np8... passed.

---------------------------------------
543_hanford_srfcplx_param...
    cd /home/gehammo/software/pflotran-dev/regression_tests/default/543
    /home/gehammo/software/pflotran-dev/src/pflotran/pflotran -malloc 0 -successful_exit_code 86 -input_prefix
543_hanford_srfcplx_param
    # 543_hanford_srfcplx_param : run time : 2.91 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]:31 : 1.76111798338e-12 > 1e-12 [relative]
    FAIL: LIQUID VELOCITY [m/d]:29 : 2.25552127701e-12 > 1e-12 [relative]
    FAIL: LIQUID VELOCITY [m/d]:29 : 1.61796082447e-11 > 1e-12 [relative]
    FAIL: UO3.2H2O SI:Min : 4.37393289458e-12 > 1e-12 [relative]
    FAIL: UO2(PO3)2 SI:Min : 4.34539859641e-12 > 1e-12 [relative]
    FAIL: UO2SO4 SI:Min : 4.32535887832e-12 > 1e-12 [relative]
    FAIL: Torbernite SI:Min : 8.7624584403e-12 > 1e-12 [relative]
    FAIL: (UO2)3(PO4)2.4H2O SI:Min : 1.30878004044e-11 > 1e-12 [relative]
    FAIL: UO2CO3 SI:Min : 4.36306510613e-12 > 1e-12 [relative]
    FAIL: UO3.0.9H2O(alpha) SI:Min : 4.37498338731e-12 > 1e-12 [relative]
    FAIL: Metatorbernite SI:Min : 8.75578249827e-12 > 1e-12 [relative]
    FAIL: CaUO4 SI:Min : 4.38494539832e-12 > 1e-12 [relative]
    FAIL: (UO2)3(PO4)2 SI:Min : 1.30887549659e-11 > 1e-12 [relative]
    FAIL: UOF4 SI:Min : 4.34665543516e-12 > 1e-12 [relative]
    FAIL: Saleeite SI:Min : 8.72937379374e-12 > 1e-12 [relative]
    FAIL: Schoepite SI:Min : 4.37393289458e-12 > 1e-12 [relative]
543_hanford_srfcplx_param... failed.
```

pflotran-tests-2016-07-29_10-27-50.testlog

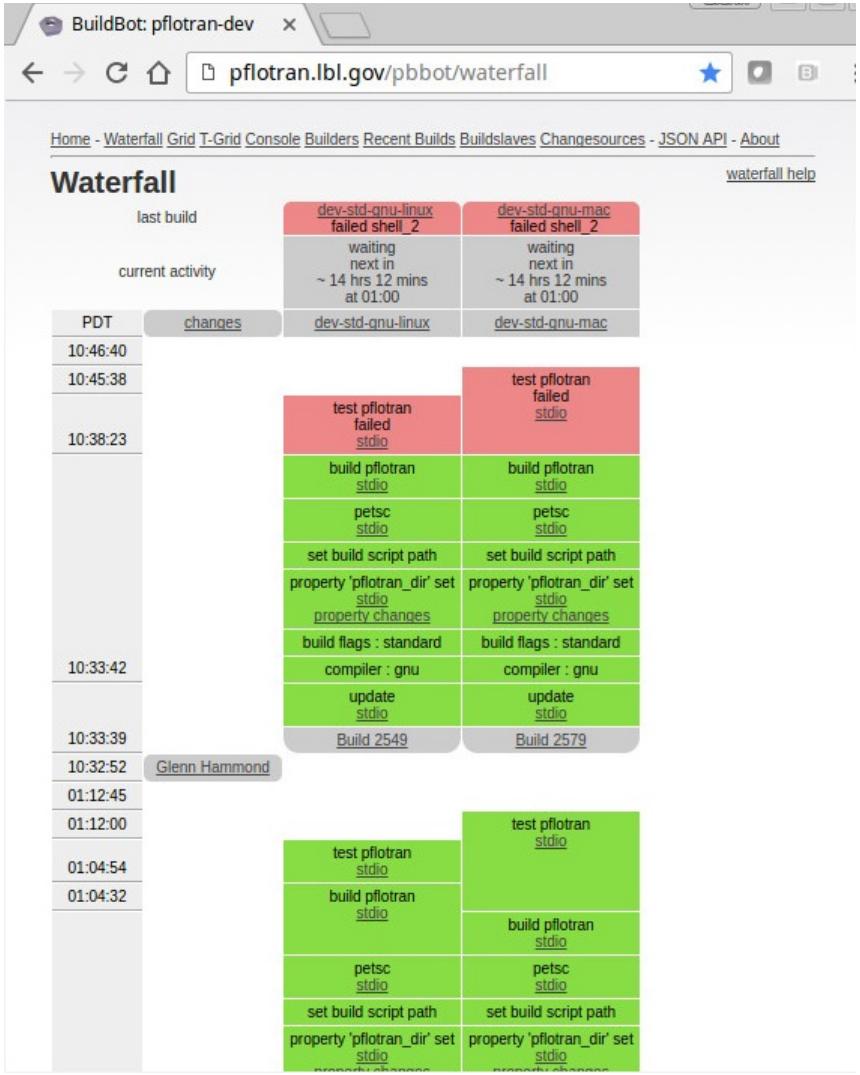
```
---------------------------------------
543_flow-np8...
    cd /home/gehammo/software/pflotran-dev/regression_tests/default/543
    /home/gehammo/local/bin/mpiexec -np 8 /home/gehammo/software/pflotran-dev/src/pflotran/pflotran -malloc 0 -
successful_exit_code 86 -input_prefix 543_flow-np8
    # 543_flow-np8 : run time : 1.31 seconds
    diff 543_flow-np8.regression.gold 543_flow-np8.regression
543_flow-np8... passed.

---------------------------------------
543_hanford_srfcplx_param...
    cd /home/gehammo/software/pflotran-dev/regression_tests/default/543
    /home/gehammo/software/pflotran-dev/src/pflotran/pflotran -malloc 0 -successful_exit_code 86 -input_prefix
543_hanford_srfcplx_param
    # 543_hanford_srfcplx_param : run time : 2.91 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]:31 : 1.76111798338e-12 > 1e-12 [relative]
    FAIL: LIQUID VELOCITY [m/d]:29 : 2.25552127701e-12 > 1e-12 [relative]
    FAIL: LIQUID VELOCITY [m/d]:29 : 1.61796082447e-11 > 1e-12 [relative]
    FAIL: UO3.2H2O SI:Min : 4.37393289458e-12 > 1e-12 [relative]
    FAIL: UO2(PO3)2 SI:Min : 4.34539859641e-12 > 1e-12 [relative]
    FAIL: UO2SO4 SI:Min : 4.32535887832e-12 > 1e-12 [relative]
    FAIL: Torbernite SI:Min : 8.7624584403e-12 > 1e-12 [relative]
    FAIL: (UO2)3(PO4)2.4H2O SI:Min : 1.30878004044e-11 > 1e-12 [relative]
    FAIL: UO2CO3 SI:Min : 4.36306510613e-12 > 1e-12 [relative]
    FAIL: UO3.0.9H2O(alpha) SI:Min : 4.37498338731e-12 > 1e-12 [relative]
    FAIL: Metatorbernite SI:Min : 8.75578249827e-12 > 1e-12 [relative]
    FAIL: CaUO4 SI:Min : 4.38494539832e-12 > 1e-12 [relative]
    FAIL: (UO2)3(PO4)2 SI:Min : 1.30887549659e-11 > 1e-12 [relative]
    FAIL: UOF4 SI:Min : 4.34665543516e-12 > 1e-12 [relative]
    FAIL: Saleeite SI:Min : 8.72937379374e-12 > 1e-12 [relative]
    FAIL: Schoepite SI:Min : 4.37393289458e-12 > 1e-12 [relative]
543_hanford_srfcplx_param... failed.
```

Buildbot: pflotran.lbl.gov/pbbot/waterfall



Mac is still testing

Buildbot: pflotran.lbl.gov/pbbot/waterfall



Code Coverage

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- Steps to generating code coverage statistics with Intel codecov
  1) Load Intel compilers
     - `source /opt/intel/bin/compilervars.csh intel64`
  2) Instrument files at compile time
     - `CC_FLAGS += -prof-gen=srcpos -prof-dir <path>`
     - `FC_FLAGS += -prof-gen=srcpos -prof-dir <path>`
  3) Run simulations
  4) Merge dynamic profile information (*.dyn) files
     - `profmerge`
  5) Generate code coverage results
     - `codecov -spi pgopti.spi -dpi pgopti.dpi`
  6) View results in `<path>/CODE_COVERAGE.HTML`

CODE_COVERAGE.HTML

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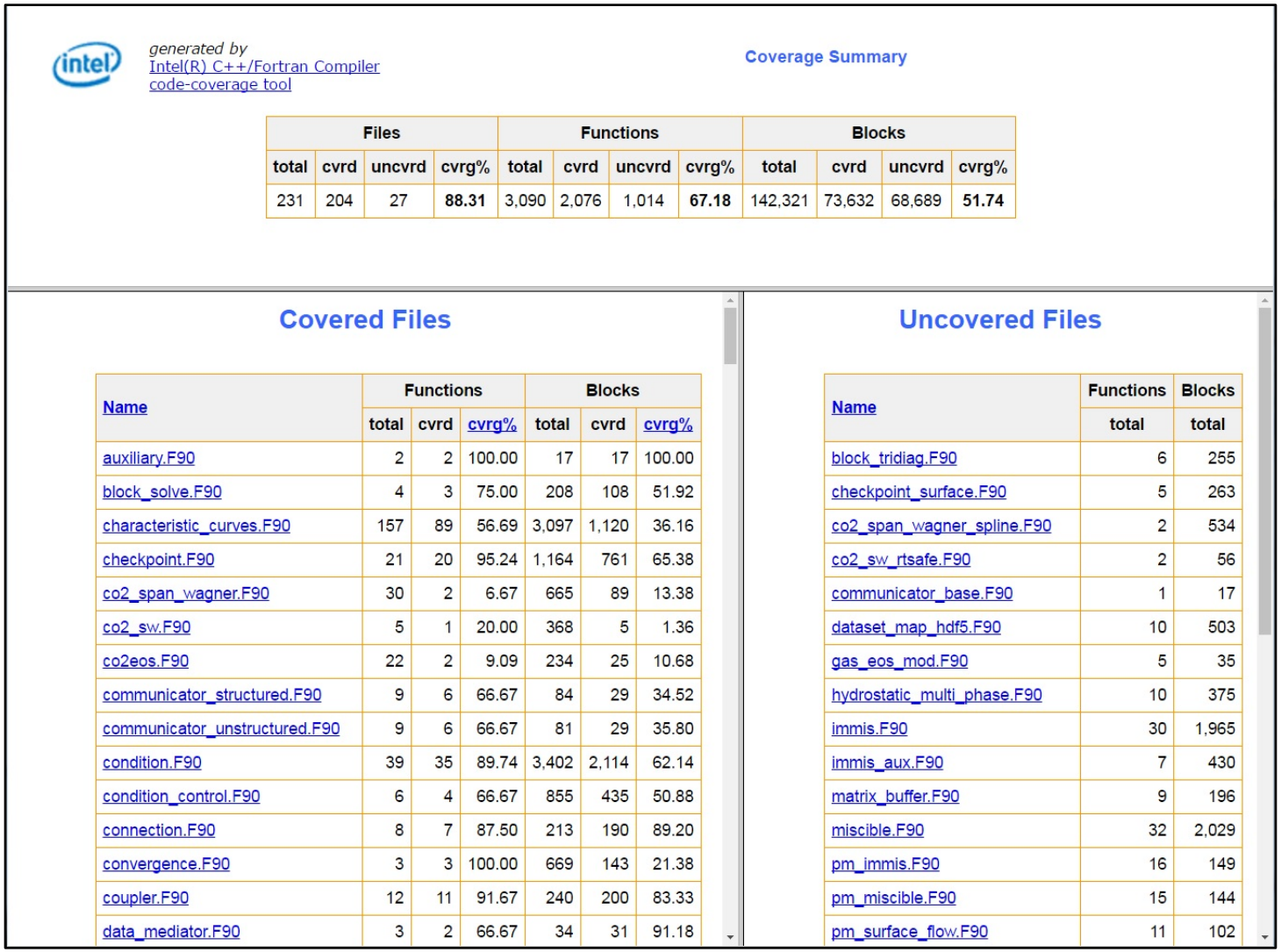

generated by
Intel(R) C++/Fortran Compiler
code-coverage tool

Coverage Summary

Files				Functions				Blocks			
total	cvrd	uncvrd	cvrg%	total	cvrd	uncvrd	cvrg%	total	cvrd	uncvrd	cvrg%
231	204	27	**88.31**	3,090	2,076	1,014	**67.18**	142,321	73,632	68,689	**51.74**

Covered Files

Name	Functions			Blocks		
	total	cvrd	cvrg%	total	cvrd	cvrg%
auxiliary.F90	2	2	100.00	17	17	100.00
block_solve.F90	4	3	75.00	208	108	51.92
characteristic_curves.F90	157	89	56.69	3,097	1,120	36.16
checkpoint.F90	21	20	95.24	1,164	761	65.38
co2_span_wagner.F90	30	2	6.67	665	89	13.38
co2_sw.F90	5	1	20.00	368	5	1.36
co2eos.F90	22	2	9.09	234	25	10.68
communicator_structured.F90	9	6	66.67	84	29	34.52
communicator_unstructured.F90	9	6	66.67	81	29	35.80
condition.F90	39	35	89.74	3,402	2,114	62.14
condition_control.F90	6	4	66.67	855	435	50.88
connection.F90	8	7	87.50	213	190	89.20
convergence.F90	3	3	100.00	669	143	21.38
coupler.F90	12	11	91.67	240	200	83.33
data_mediator.F90	3	2	66.67	34	31	91.18

Uncovered Files

Name	Functions	Blocks
	total	total
block_tridiag.F90	6	255
checkpoint_surface.F90	5	263
co2_span_wagner_spline.F90	2	534
co2_sw_rtsafe.F90	2	56
communicator_base.F90	1	17
dataset_map_hdf5.F90	10	503
gas_eos_mod.F90	5	35
hydrostatic_multi_phase.F90	10	375
immis.F90	30	1,965
immis_aux.F90	7	430
matrix_buffer.F90	9	196
miscible.F90	32	2,029
pm_immis.F90	16	149
pm_miscible.F90	15	144
pm_surface_flow.F90	11	102

CODE_COVERAGE.HTML

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Files				Fu	
total	cvrd	uncvrd	cvrg%	total	cvrd
231	204	27	88.31	3,090	2,076

- Intel codecov
  - Poor coverage
    - dataset_map_hdf5.F90
  - Good coverage
    - material.F90
  - Excellent coverage
    - srcsink_sandbox_wipp_gas.

Name
material.F90

Uncovered Files

Name	Functions	Blocks
	total	total
block_tridiag.F90	6	255
checkpoint_surface.F90	5	263
co2_span_wagner_spline.F90	2	534
co2_sw_rtsafe.F90	2	56
communicator_base.F90	1	17
dataset_map_hdf5.F90	10	503
gas_eos_mod.F90	5	35
hydrostatic_multi_phase.F90	10	375

Name	Functions			Blocks		
	total	cvrd	cvrg%	total	cvrd	cvrg%
srcsink_sandbox_wipp_gas.F90	5	5	100.00	68	67	98.53

dataset_map_hdf5.F90

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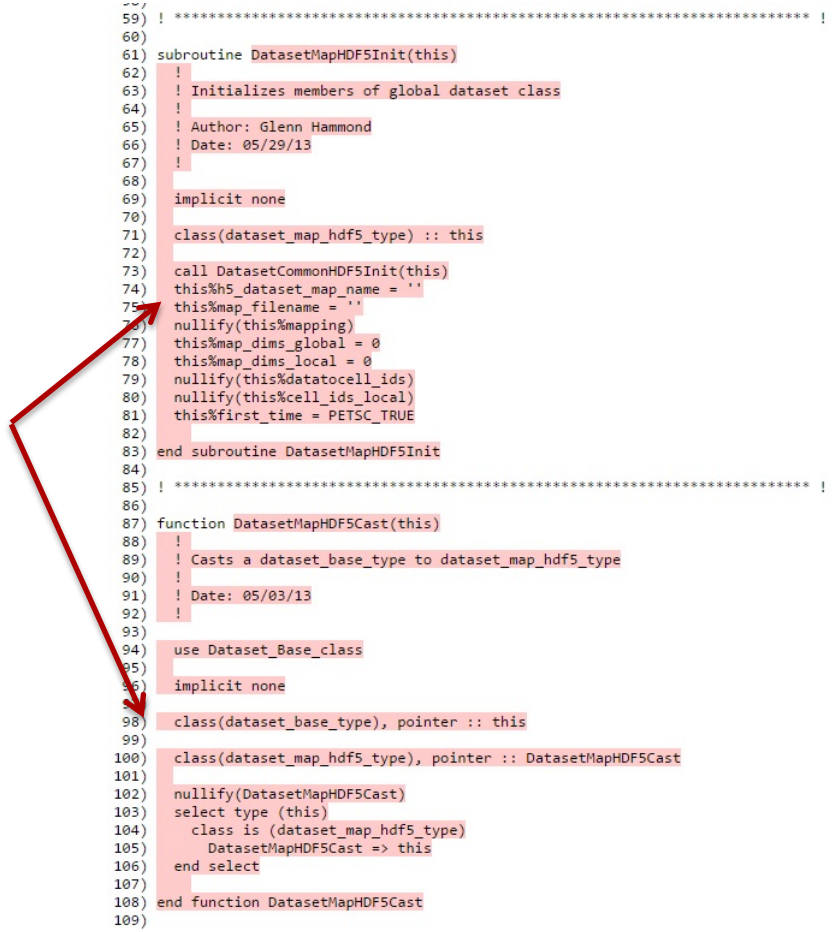
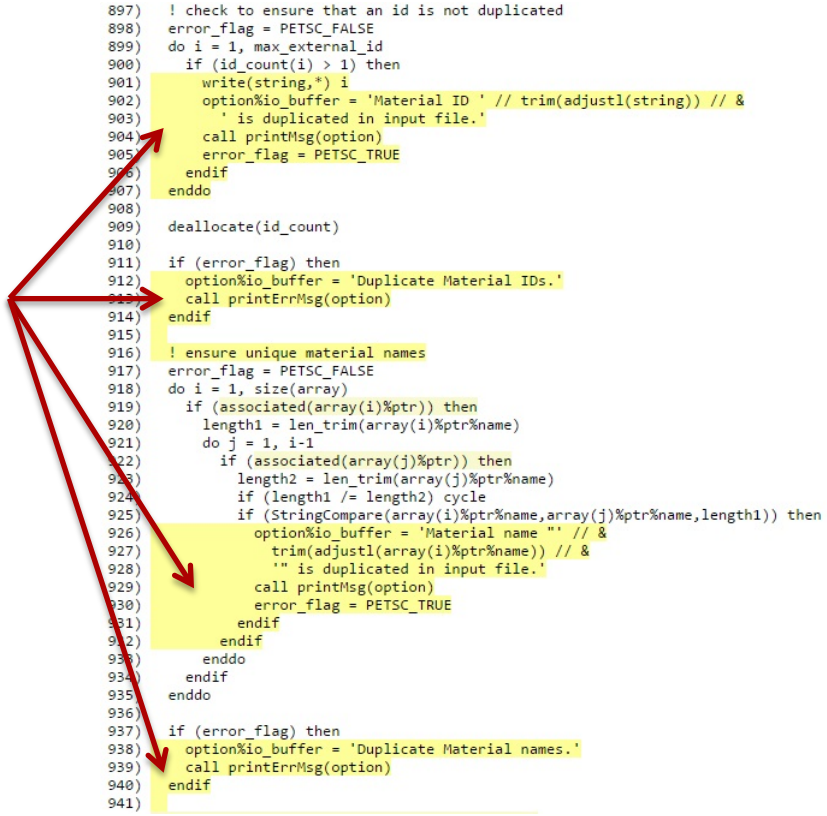
Uncovered subroutines



```
59) ! ************************************************************************** !
60)
61) subroutine DatasetMapHDF5Init(this)
62)   !
63)   ! Initializes members of global dataset class
64)   !
65)   ! Author: Glenn Hammond
66)   ! Date: 05/29/13
67)   !
68)
69)   implicit none
70)
71)   class(dataset_map_hdf5_type) :: this
72)
73)   call DatasetCommonHDF5Init(this)
74)   this%h5_dataset_map_name = ''
75)   this%map_filename = ''
76)   nullify(this%mapping)
77)   this%map_dims_global = 0
78)   this%map_dims_local = 0
79)   nullify(this%datatocell_ids)
80)   nullify(this%cell_ids_local)
81)   this%first_time = PETSC_TRUE
82)
83) end subroutine DatasetMapHDF5Init
84)
85) ! ************************************************************************** !
86)
87) function DatasetMapHDF5Cast(this)
88)   !
89)   ! Casts a dataset_base_type to dataset_map_hdf5_type
90)   !
91)   ! Date: 05/03/13
92)   !
93)
94)   use Dataset_Base_class
95)
96)   implicit none
97)
98)   class(dataset_base_type), pointer :: this
99)
100)   class(dataset_map_hdf5_type), pointer :: DatasetMapHDF5Cast
101)
102)   nullify(DatasetMapHDF5Cast)
103)   select type (this)
104)     class is (dataset_map_hdf5_type)
105)       DatasetMapHDF5Cast => this
106)   end select
107)
108) end function DatasetMapHDF5Cast
109)
```

material.F90

Error messaging



```
897)   ! check to ensure that an id is not duplicated
898)   error_flag = PETSC_FALSE
899)   do i = 1, max_external_id
900)     if (id_count(i) > 1) then
901)       write(string,*) i
902)       option%io_buffer = 'Material ID ' // trim(adjustl(string)) // &
903)         ' is duplicated in input file.'
904)       call printMsg(option)
905)       error_flag = PETSC_TRUE
906)     endif
907)   enddo
908)
909)   deallocate(id_count)
910)
911)   if (error_flag) then
912)     option%io_buffer = 'Duplicate Material IDs.'
913)     call printErrMsg(option)
914)   endif
915)
916)   ! ensure unique material names
917)   error_flag = PETSC_FALSE
918)   do i = 1, size(array)
919)     if (associated(array(i)%ptr)) then
920)       length1 = len_trim(array(i)%ptr%name)
921)       do j = 1, i-1
922)         if (associated(array(j)%ptr)) then
923)           length2 = len_trim(array(j)%ptr%name)
924)           if (length1 /= length2) cycle
925)           if (StringCompare(array(i)%ptr%name,array(j)%ptr%name,length1)) then
926)             option%io_buffer = 'Material name "' // &
927)               trim(adjustl(array(i)%ptr%name)) // &
928)               '" is duplicated in input file.'
929)             call printMsg(option)
930)             error_flag = PETSC_TRUE
931)           endif
932)         endif
933)       enddo
934)     endif
935)   enddo
936)
937)   if (error_flag) then
938)     option%io_buffer = 'Duplicate Material names.'
939)     call printErrMsg(option)
940)   endif
941)
```

material.F90

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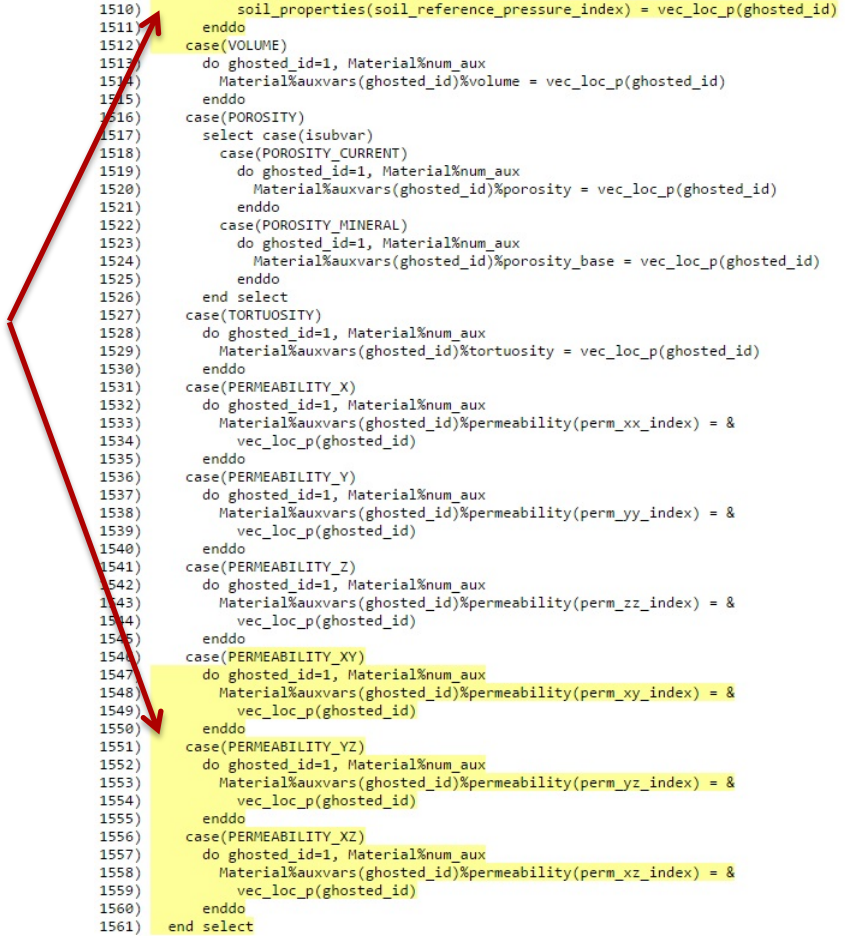
Uncovered code blocks



```
1501)   select case(ivar)
1502)     case(SOIL_COMPRESSIBILITY)
1503)       do ghosted_id=1, Material%num_aux
1504)         Material%auxvars(ghosted_id)% &
1505)           soil_properties(soil_compressibility_index) = vec_loc_p(ghosted_id)
1506)       enddo
1507)     case(SOIL_REFERENCE_PRESSURE)
1508)       do ghosted_id=1, Material%num_aux
1509)         Material%auxvars(ghosted_id)% &
1510)           soil_properties(soil_reference_pressure_index) = vec_loc_p(ghosted_id)
1511)       enddo
1512)     case(VOLUME)
1513)       do ghosted_id=1, Material%num_aux
1514)         Material%auxvars(ghosted_id)%volume = vec_loc_p(ghosted_id)
1515)       enddo
1516)     case(POROSITY)
1517)       select case(isubvar)
1518)         case(POROSITY_CURRENT)
1519)           do ghosted_id=1, Material%num_aux
1520)             Material%auxvars(ghosted_id)%porosity = vec_loc_p(ghosted_id)
1521)           enddo
1522)         case(POROSITY_MINERAL)
1523)           do ghosted_id=1, Material%num_aux
1524)             Material%auxvars(ghosted_id)%porosity_base = vec_loc_p(ghosted_id)
1525)           enddo
1526)       end select
1527)     case(TORTUOSITY)
1528)       do ghosted_id=1, Material%num_aux
1529)         Material%auxvars(ghosted_id)%tortuosity = vec_loc_p(ghosted_id)
1530)       enddo
1531)     case(PERMEABILITY_X)
1532)       do ghosted_id=1, Material%num_aux
1533)         Material%auxvars(ghosted_id)%permeability(perm_xx_index) = &
1534)           vec_loc_p(ghosted_id)
1535)       enddo
1536)     case(PERMEABILITY_Y)
1537)       do ghosted_id=1, Material%num_aux
1538)         Material%auxvars(ghosted_id)%permeability(perm_yy_index) = &
1539)           vec_loc_p(ghosted_id)
1540)       enddo
1541)     case(PERMEABILITY_Z)
1542)       do ghosted_id=1, Material%num_aux
1543)         Material%auxvars(ghosted_id)%permeability(perm_zz_index) = &
1544)           vec_loc_p(ghosted_id)
1545)       enddo
1546)     case(PERMEABILITY_XY)
1547)       do ghosted_id=1, Material%num_aux
1548)         Material%auxvars(ghosted_id)%permeability(perm_xy_index) = &
1549)           vec_loc_p(ghosted_id)
1550)       enddo
1551)     case(PERMEABILITY_YZ)
1552)       do ghosted_id=1, Material%num_aux
1553)         Material%auxvars(ghosted_id)%permeability(perm_yz_index) = &
1554)           vec_loc_p(ghosted_id)
1555)       enddo
1556)     case(PERMEABILITY_XZ)
1557)       do ghosted_id=1, Material%num_aux
1558)         Material%auxvars(ghosted_id)%permeability(perm_xz_index) = &
1559)           vec_loc_p(ghosted_id)
1560)       enddo
1561)   end select
```

material.F90

Sandia National Laboratories

Uncovered subroutine

```
1816) subroutine MaterialUpdatePorosity(Material,global_auxvars,porosity_loc)
1817)   !
1818)   ! Gets values of material auxvar data using a vector.
1819)   !
1820)   ! Author: Glenn Hammond
1821)   ! Date: 01/09/14
1822)   !
1823)
1824)   use Variables_module
1825)   use Global_Aux_module
1826)
1827)   implicit none
1828)
1829) #include "petsc/finclude/petscvec.h"
1830) #include "petsc/finclude/petscvec.h90"
1831)
1832)   type(material_type) :: Material ! from realization%patch%aux%Material
1833)   type(global_auxvar_type) :: global_auxvars(:)
1834)   Vec :: porosity_loc
1835)
1836)   PetscReal, pointer :: porosity_loc_p(:)
1837)   class(material_auxvar_type), pointer :: material_auxvars(:)
1838)   PetscInt :: ghosted_id
1839)   PetscReal :: compressed_porosity
1840)   PetscReal :: dcompressed_porosity_dp
1841)   PetscErrorCode :: ierr
1842)
1843)   if (soil_compressibility_index > 0) then
1844)     material_auxvars => Material%auxvars
1845)     call VecGetArrayReadF90(porosity_loc,porosity_loc_p,ierr);CHKERRQ(ierr)
1846)     do ghosted_id = 1, Material%num_aux
1847)       material_auxvars(ghosted_id)%porosity = porosity_loc_p(ghosted_id)
1848)       call MaterialCompressSoil(material_auxvars(ghosted_id), &
1849)                                 maxval(global_auxvars(ghosted_id)%pres), &
1850)                                 compressed_porosity,dcompressed_porosity_dp)
1851)       material_auxvars(ghosted_id)%porosity = compressed_porosity
1852)       material_auxvars(ghosted_id)%dporosity_dp = dcompressed_porosity_dp
1853)     enddo
1854)     call VecRestoreArrayReadF90(porosity_loc,porosity_loc_p, &
1855)                                 ierr);CHKERRQ(ierr)
1856)   endif
1857)
1858) end subroutine MaterialUpdatePorosity
```

srcsink_sandbox_wipp_gas.F90

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```
64) subroutine WIPPGasGenerationRead(this,input,option)
65)   !
66)   ! Reads input deck for WIPP gas generation src/sink parameters
67)   !
68)   ! Author: Glenn Hammond, Edit: Heeho Park
69)   ! Date: 04/11/14, 05/15/14
70)   !
71)
72)   use Option_module
73)   use String_module
74)   use Input_Aux_module
75)   use Units_module, only : UnitsConvertToInternal
76)
77)   implicit none
78)
79)   class(srcsink_sandbox_wipp_gas_type) :: this
80)   type(input_type), pointer :: input
81)   type(option_type) :: option
82)
83)   PetscInt :: i
84)   character(len=MAXWORDLENGTH) :: word, internal_units
85)   PetscBool :: found
86)
87)   do
88)     call InputReadPflotranString(input,option)
89)     if (InputError(input)) exit
90)     if (InputCheckExit(input,option)) exit
91)
92)     call InputReadWord(input,option,word,PETSC_TRUE)
93)     call InputErrorMsg(input,option,'keyword', &
94)                        'SRCSINK_SANDBOX,WIPP')
95)     call StringToUpper(word)
96)
97)     call SSSandboxBaseSelectCase(this,input,option,word,found)
98)     if (found) cycle
99)
100)    select case(trim(word))
101)      case('INUNDATED_CORROSION_RATE')
102)        internal_units = 'unitless/sec'
103)        call InputReadDouble(input,option,this%inundated_corrosion_rate)
104)        call InputDefaultMsg(input,option,'inundated_corrosion_rate')
105)      case('INUNDATED_DEGRADATION_RATE')
106)        internal_units = 'unitless/sec'
107)        call InputReadDouble(input,option,this%inundated_degradation_rate)
108)        call InputDefaultMsg(input,option,'inundated_degradation_rate')
109)      case('HUMID_CORROSION_FACTOR')
110)        call InputReadDouble(input,option,this%humid_corrosion_factor)
111)        call InputDefaultMsg(input,option,'humid_corrosion_factor')
112)      case('HUMID_DEGREDATION_FACTOR')
113)        call InputReadDouble(input,option,this%humid_degradation_factor)
114)        call InputDefaultMsg(input,option,'humid_degradation_factor')
115)      case('H2_FE_RATIO')
116)        call InputReadDouble(input,option,this%h2_fe_ratio)
117)        call InputDefaultMsg(input,option,'h2_fe_ratio')
118)      case('H2_CH2O_RATIO')
119)        call InputReadDouble(input,option,this%h2_ch2o_ratio)
120)        call InputDefaultMsg(input,option,'h2_ch2o_ratio')
121)      case default
122)        call InputKeywordUnrecognized(word, &
123)          'SRCSINK_SANDBOX,WIPP-GAS_GENERATION',option)
124)    end select
125)  enddo
126)
127) end subroutine WIPPGasGenerationRead
```

Error message

Graphical Debuggers (A Must!)

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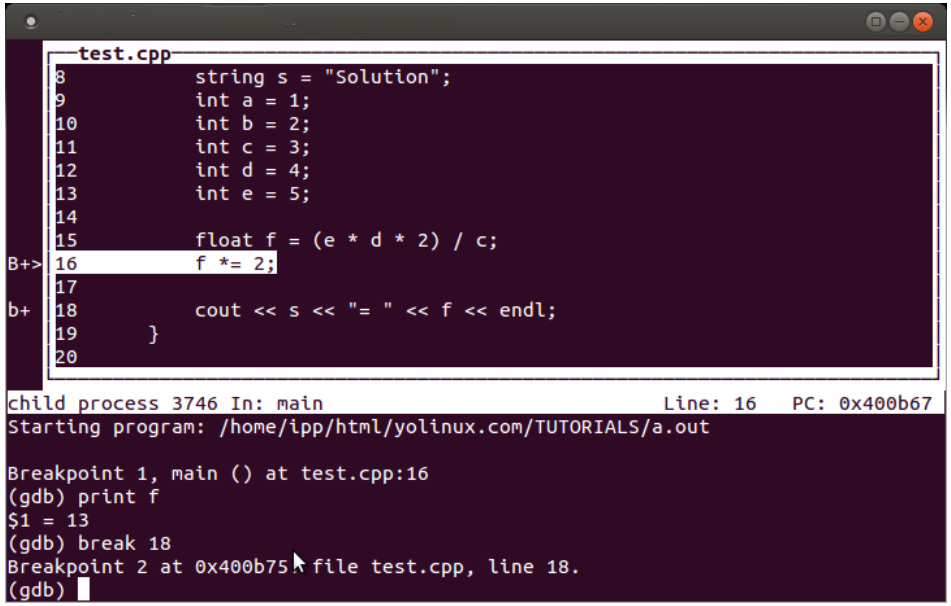
- Debugging with gdb or print statements is a thing of the past.
- Use a graphical debugger
  - Allinea DDT
  - RogueWave TotalView
  - Visual Studio
- Memory debugging
  - Intel Inspector
  - Valgrind



Debugging with two Allinea DDT debuggers

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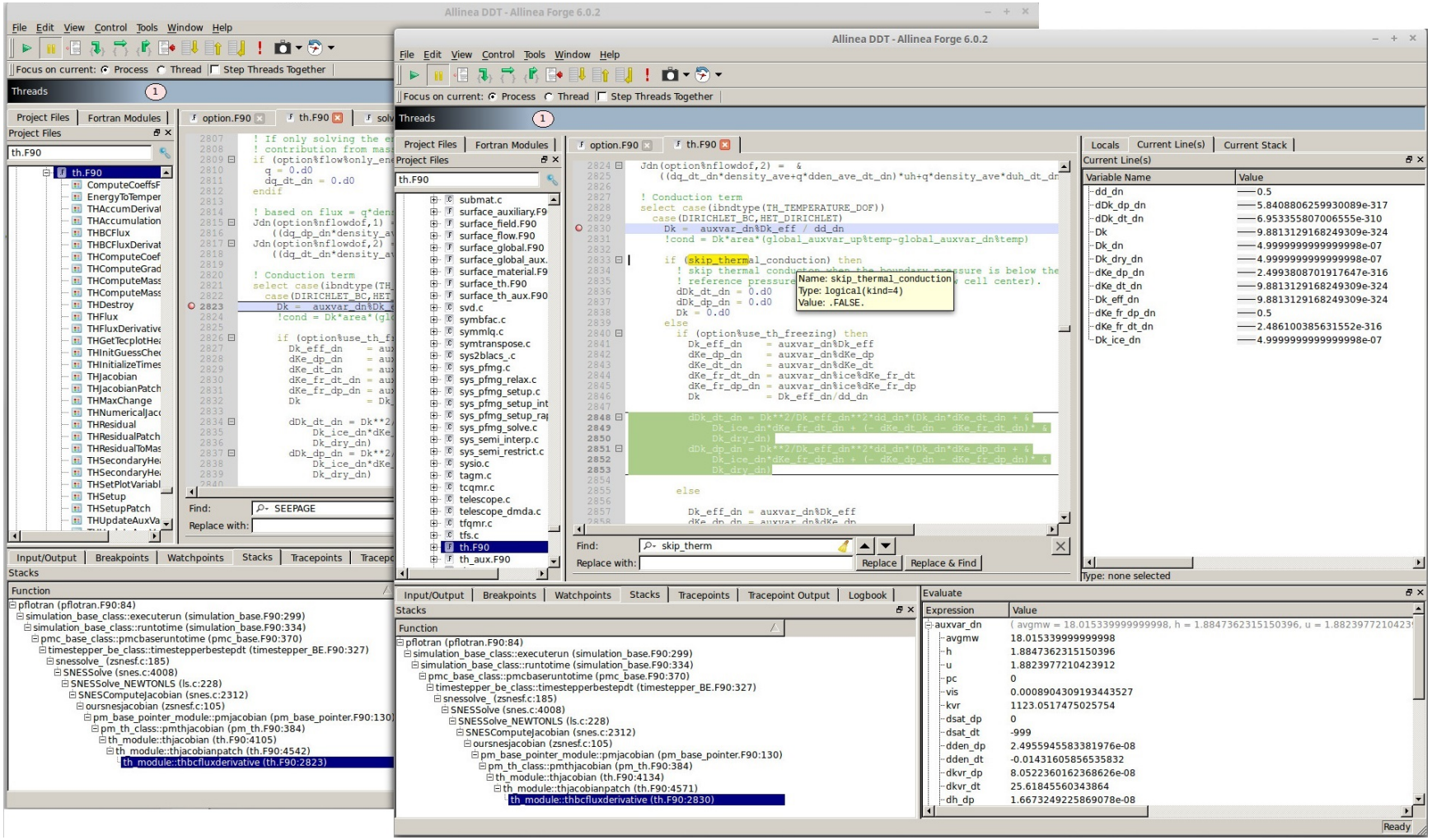

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OPEN SOURCE DEVELOPMENT

Community vs. Open Source Codes

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- A *community* of users grows around a *fit* code.
  - "Community" does not imply "open source".
  - "Open source" does not imply a "community".
- Successful open source codes tend to be governed by benevolent dictators that address and protect the needs of the entire community while accommodating the desires of individuals.
- The community can drive the code to evolve beyond the original vision (evolution).

Advantages of Open Source

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- Encourages collaboration
  - Development
  - Testing
  - Debugging
- Transparency exposes implementation details critical to scientific reproducibility, but excluded by journal publications.
- More optimal use of funding
  - Funding is pooled across a diverse set of projects/budgets.
  - What would have been spend on licensing fees can be redirected towards development.
  - Infinite benefit to those who are unfunded.
- The most fit codes tend to survive (natural selection).

Potential Disadvantages of Open Source

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- Potential time sinks
  - Newbies
  - Lookie-loos
- Care must be taken to avoid exposing the details of unpublished research.
- One's own capability can be leveraged against oneself by competitors (competing proposals).
- Dissention among the ranks (permanently forked repositories).
- Codes can be licensed as open source, but the source code remains inaccessible (disingenuous licensing).

PFLOTRAN Support Infrastructure

Sandia National Laboratories

- 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)
  - Pull requests
  - Issue tracker
- Buildbot: automated building and testing (regression and unit)
- Google Groups: pflotran-users and pflotran-dev mailing lists
- Google Analytics: tracks behavior on Bitbucket

PFLOTRAN Documentation

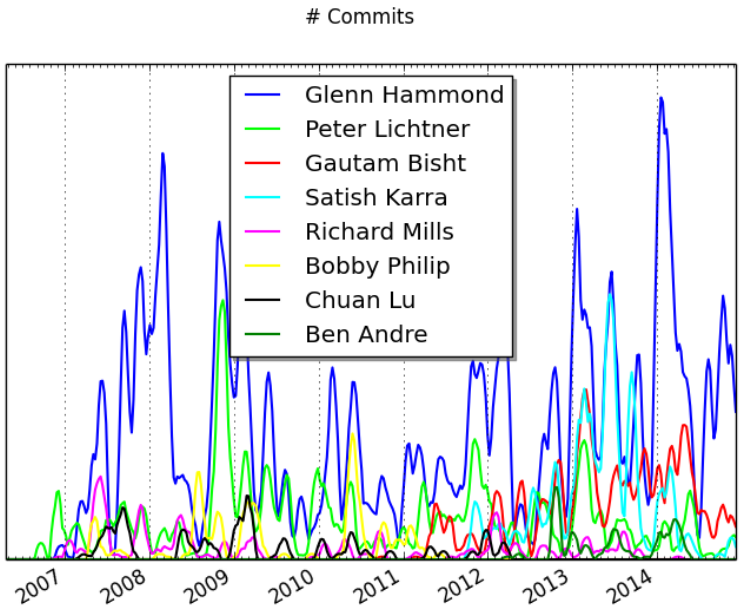
Sandia National Laboratories

- Current
  - User manual stored in code repository (LaTeX)
  - Design docs stored in separate protected repository (LaTeX)
  - Bitbucket wiki for quick guide (description of input deck cards)
- Future
  - Prototyped
    - Markdown / MkDocs
    - reStructuredTest / Sphinx
  - Planned approach
    - reStructuredText and Sphinx to generate html and pdf to be hosted on pflotran.org
    - Use converter to adapt in the future (e.g. Pandoc)

Comments on Mercurial Distributed Source Control Management

Sandia National Laboratories

- Git vs. Mercurial
  - Mercurial tends to be more novice friendly.
  - Git is clearly more popular. But as long as Mercurial continues to satisfy our needs, why change?
- Functionality
  - `hg revert`
  - `hg bisect`
  - hgactivity extension

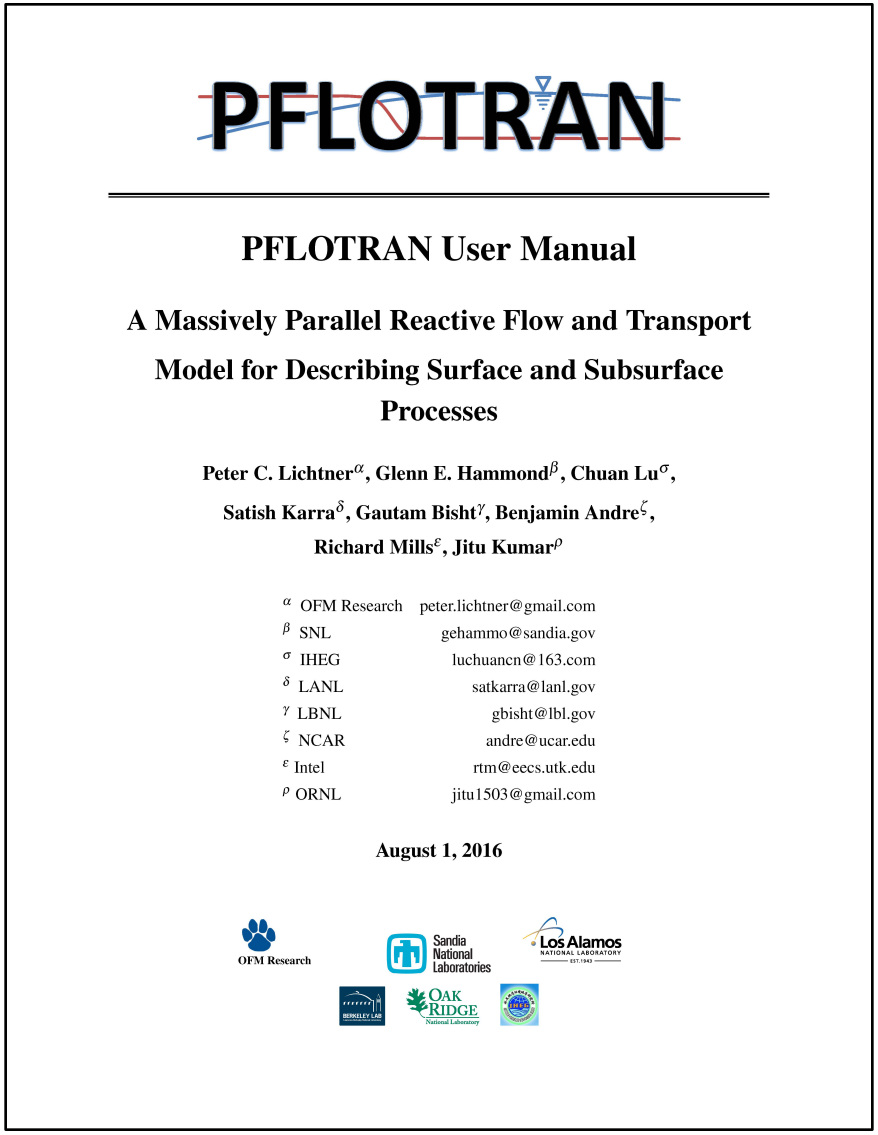


commits from 2007-2014.

PFLOTRAN User Manual

Sandia National Laboratories

LaTeX stored in PFLOTRAN code repository



PFLOTRAN

PFLOTRAN User Manual

A Massively Parallel Reactive Flow and Transport Model for Describing Surface and Subsurface Processes

Peter C. Lichtner[α], Glenn E. Hammond[β], Chuan Lu[σ], Satish Karra[δ], Gautam Bisht[γ], Benjamin Andre[ζ], Richard Mills[ε], Jitu Kumar[ρ]

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August 1, 2016

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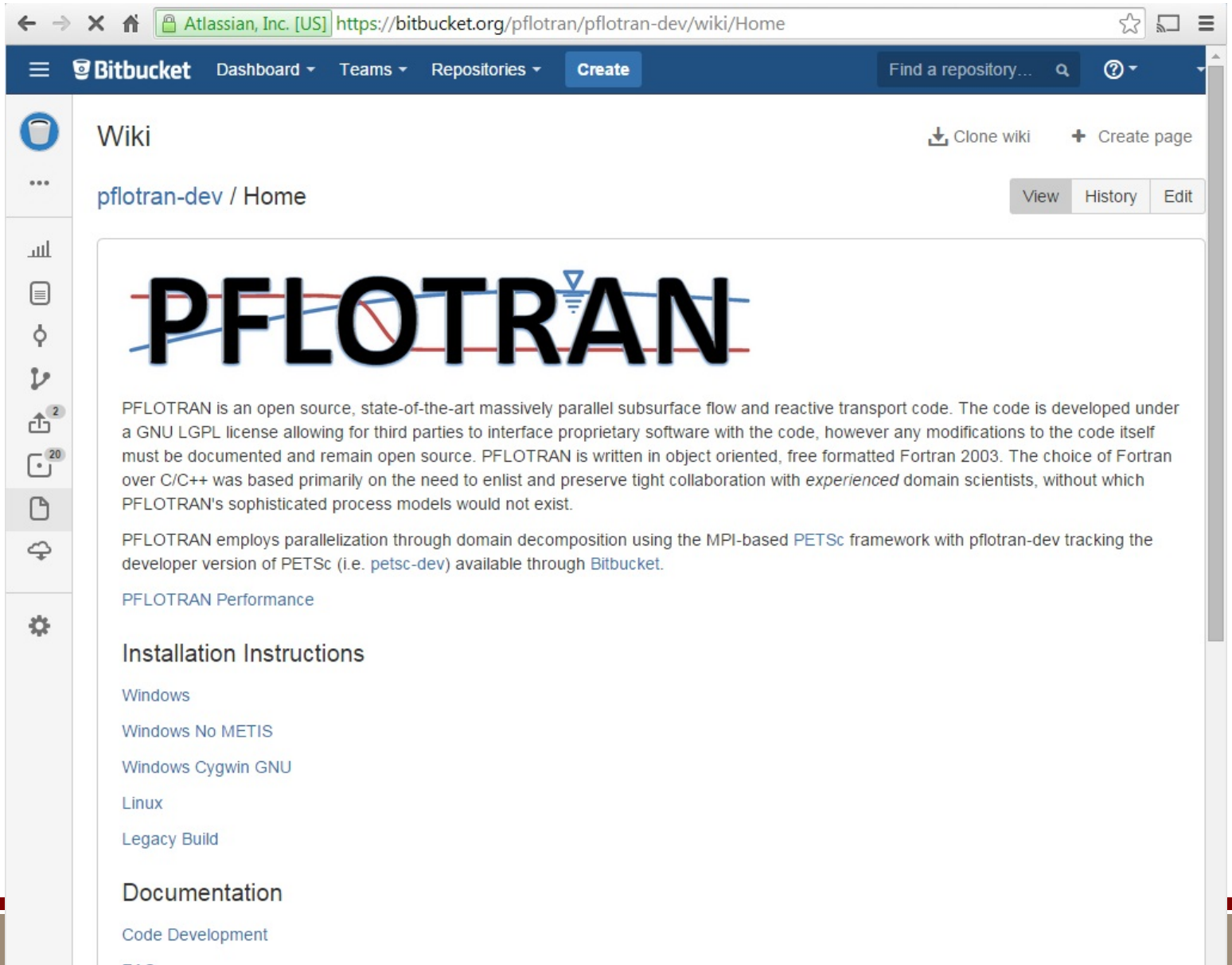
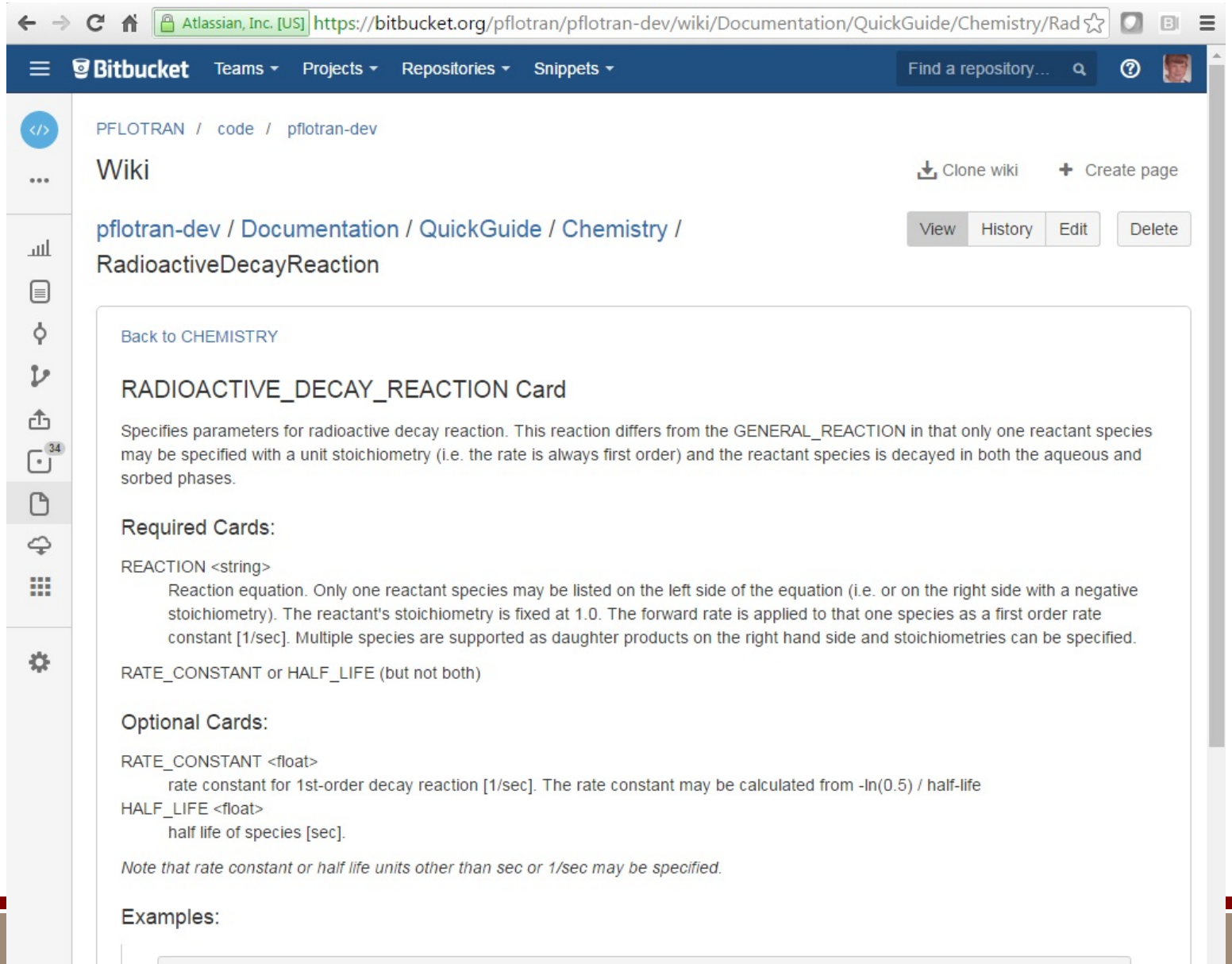
PFLOTRAN Bitbucket Site



PFLOTRAN Quick Guide

Sandia National Laboratories



PFLOTRAN Quick Guide (cont.)

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Optional Cards:

RATE_CONSTANT <float>
rate constant for 1st-order decay reaction [1/sec]. The rate constant may be calculated from -ln(0.5) / half-life
HALF_LIFE <float>
half life of species [sec].

Note that rate constant or half life units other than sec or 1/sec may be specified.

Examples:

```
RADIOACTIVE_DECAY_REACTION
  REACTION Tracer <-> Tracer2
  RATE_CONSTANT 1.7584d-7 ! half life at 0.125 y
/
```

```
CHEMISTRY
  PRIMARY_SPECIES
    A(aq)
    B(aq)
    C(aq)
  /
  ...
  RADIOACTIVE_DECAY_REACTION
    REACTION A(aq) <-> B(aq)
    ! Calculating forward rate from half-life
    ! rate = -ln(0.5) / half-life [1/sec]
    RATE_CONSTANT 1.75836d-9  ! 1/s  half life = 12.5 yrs
  /
  RADIOACTIVE_DECAY_REACTION
    REACTION B(aq) <-> C(aq)
    RATE_CONSTANT 8.7918d-10  ! 1/s  half life = 25. yrs
  /
  RADIOACTIVE_DECAY_REACTION
    ! Note that C(aq) simply decays with no daughter products
    REACTION C(aq) <->
    HALF_LIFE 5. y
  /
  ...
/
```

Updated 2015-10-30

PFLOTRAN Bitbucket Commit Log

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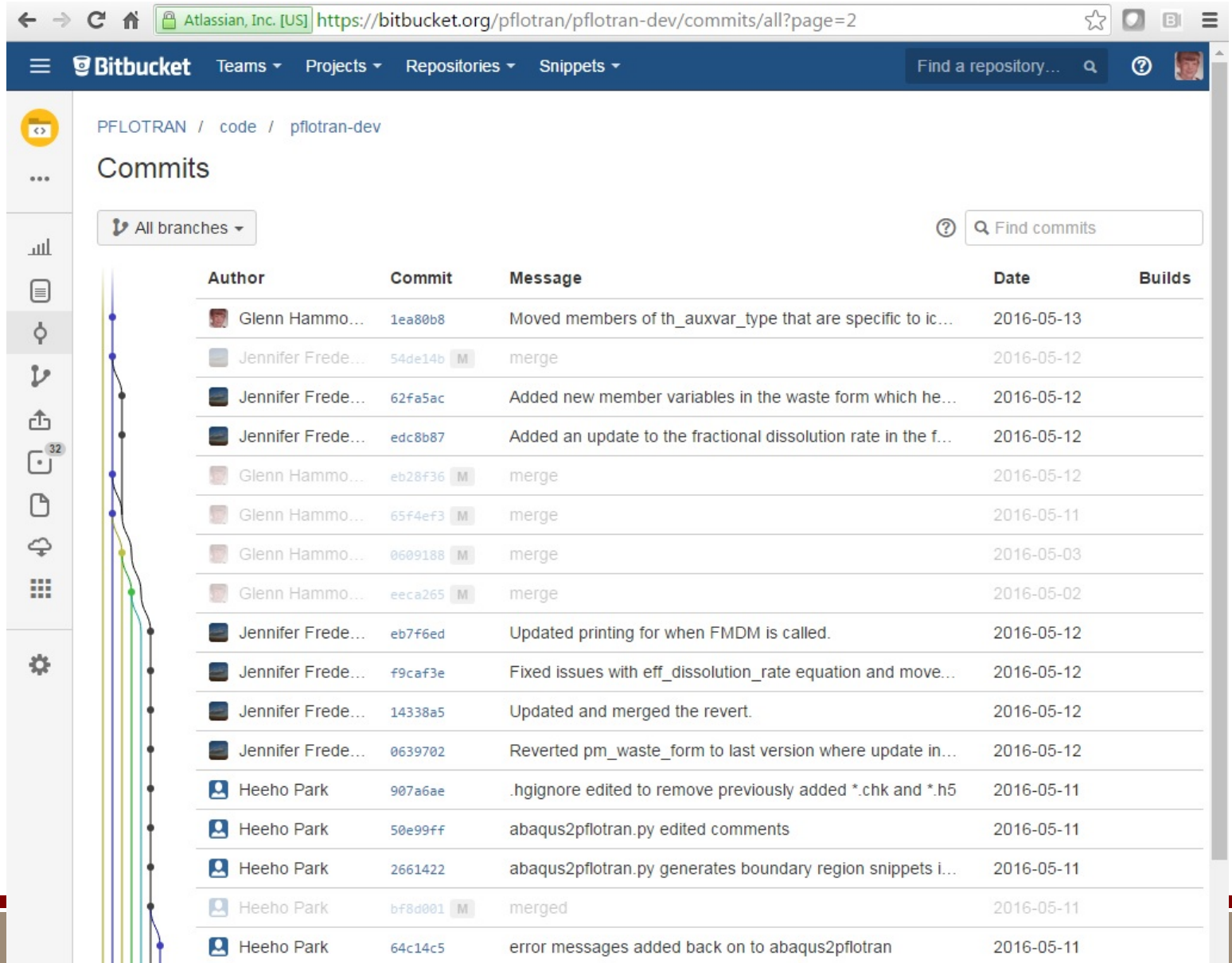

Author	Commit	Message	Date	Builds
Glenn Hammo...	1ea80b8	Moved members of th_auxvar_type that are specific to ic...	2016-05-13	
Jennifer Frede...	54de14b M	merge	2016-05-12	
Jennifer Frede...	62fa5ac	Added new member variables in the waste form which he...	2016-05-12	
Jennifer Frede...	edc8b87	Added an update to the fractional dissolution rate in the f...	2016-05-12	
Glenn Hammo...	eb28f36 M	merge	2016-05-12	
Glenn Hammo...	65f4ef3 M	merge	2016-05-11	
Glenn Hammo...	0609188 M	merge	2016-05-03	
Glenn Hammo...	eeca265 M	merge	2016-05-02	
Jennifer Frede...	eb7f6ed	Updated printing for when FMDM is called.	2016-05-12	
Jennifer Frede...	f9caf3e	Fixed issues with eff_dissolution_rate equation and move...	2016-05-12	
Jennifer Frede...	14338a5	Updated and merged the revert.	2016-05-12	
Jennifer Frede...	0639702	Reverted pm_waste_form to last version where update in...	2016-05-12	
Heeho Park	907a6ae	.hgignore edited to remove previously added *.chk and *.h5	2016-05-11	
Heeho Park	50e99ff	abaqus2pflotran.py edited comments	2016-05-11	
Heeho Park	2661422	abaqus2pflotran.py generates boundary region snippets i...	2016-05-11	
Heeho Park	bf8d001 M	merged	2016-05-11	
Heeho Park	64c14c5	error messages added back on to abaqus2pflotran	2016-05-11	

PFLOTRAN Bitbucket Commit

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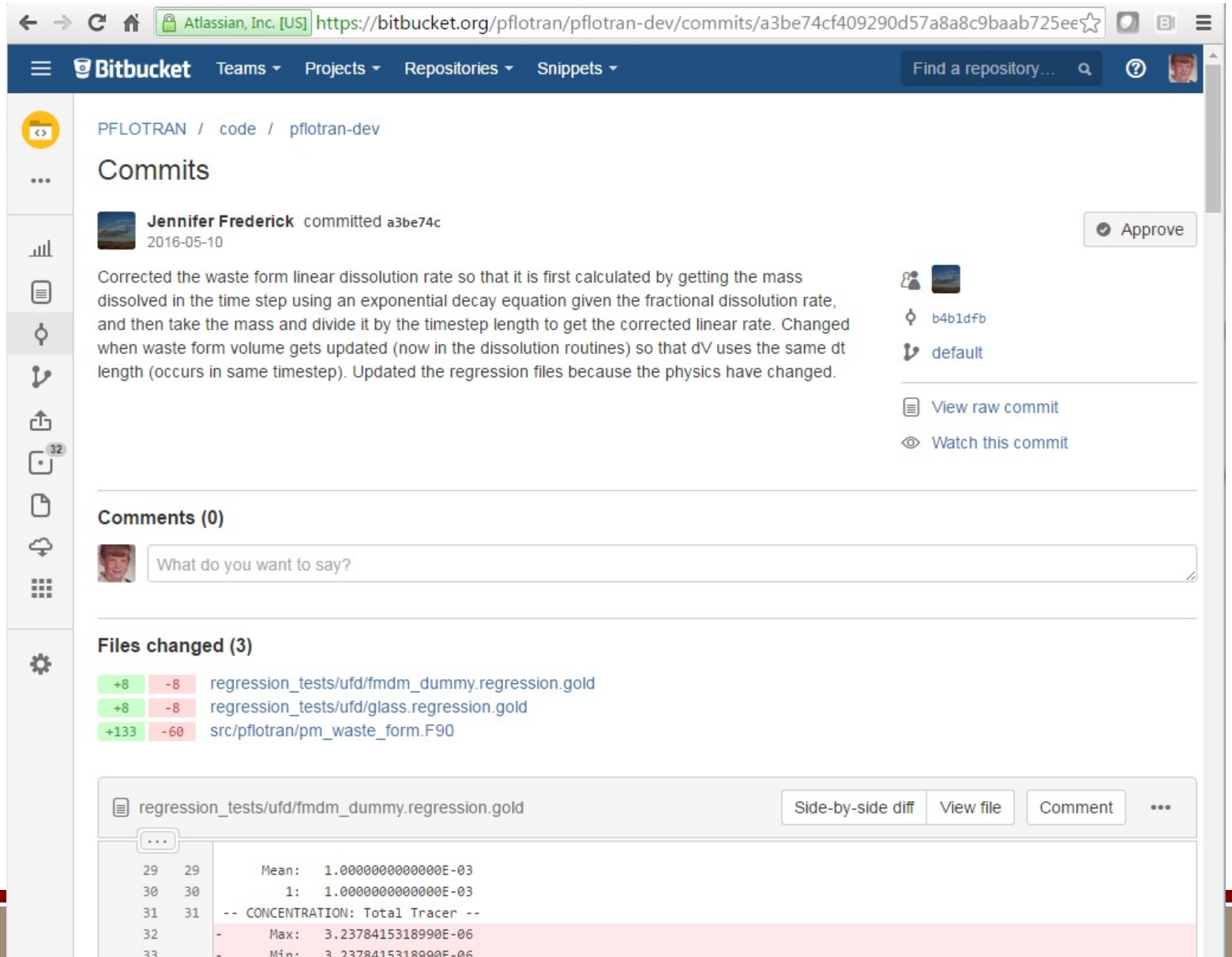

PFLOTRAN Bitbucket Pull Request

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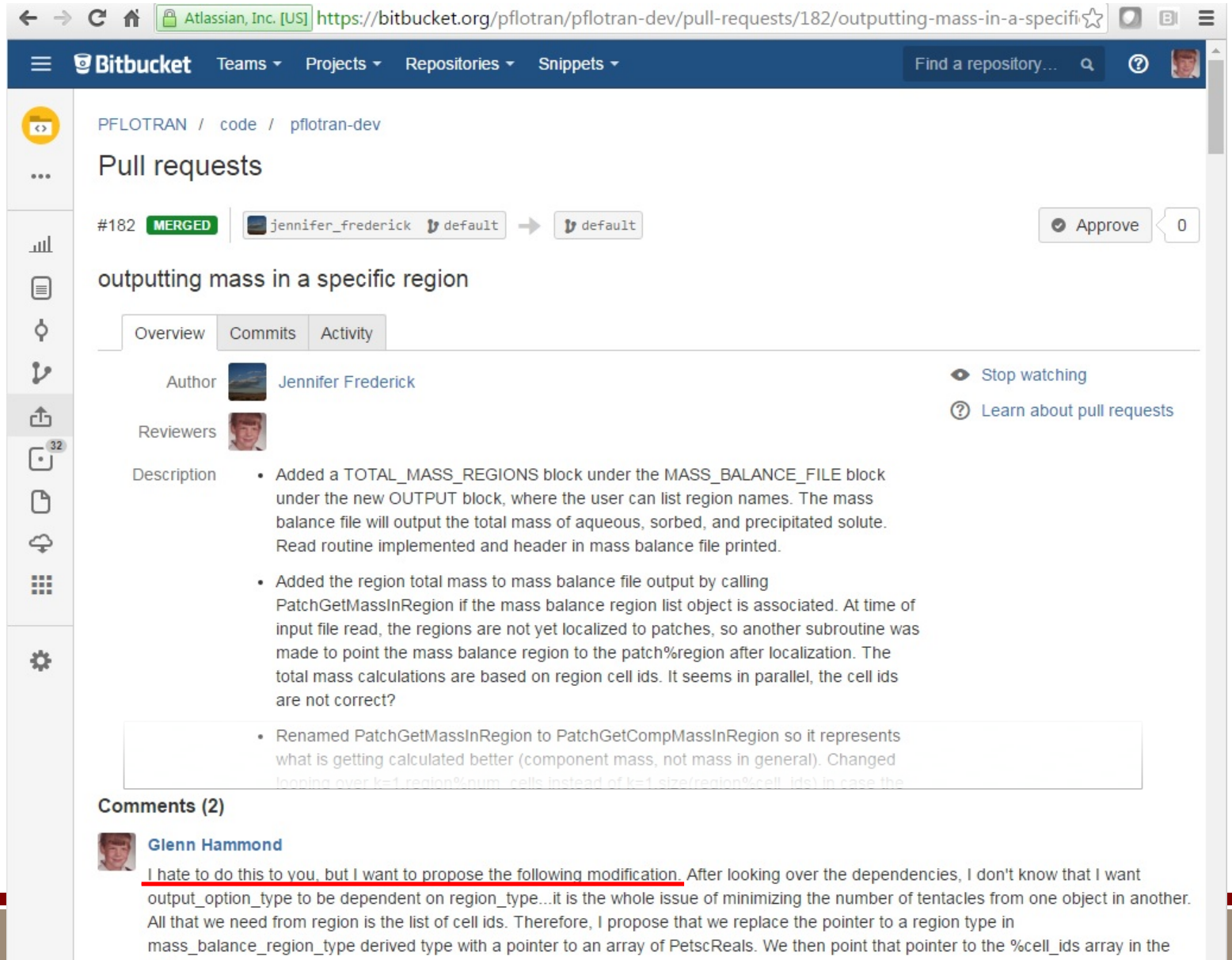
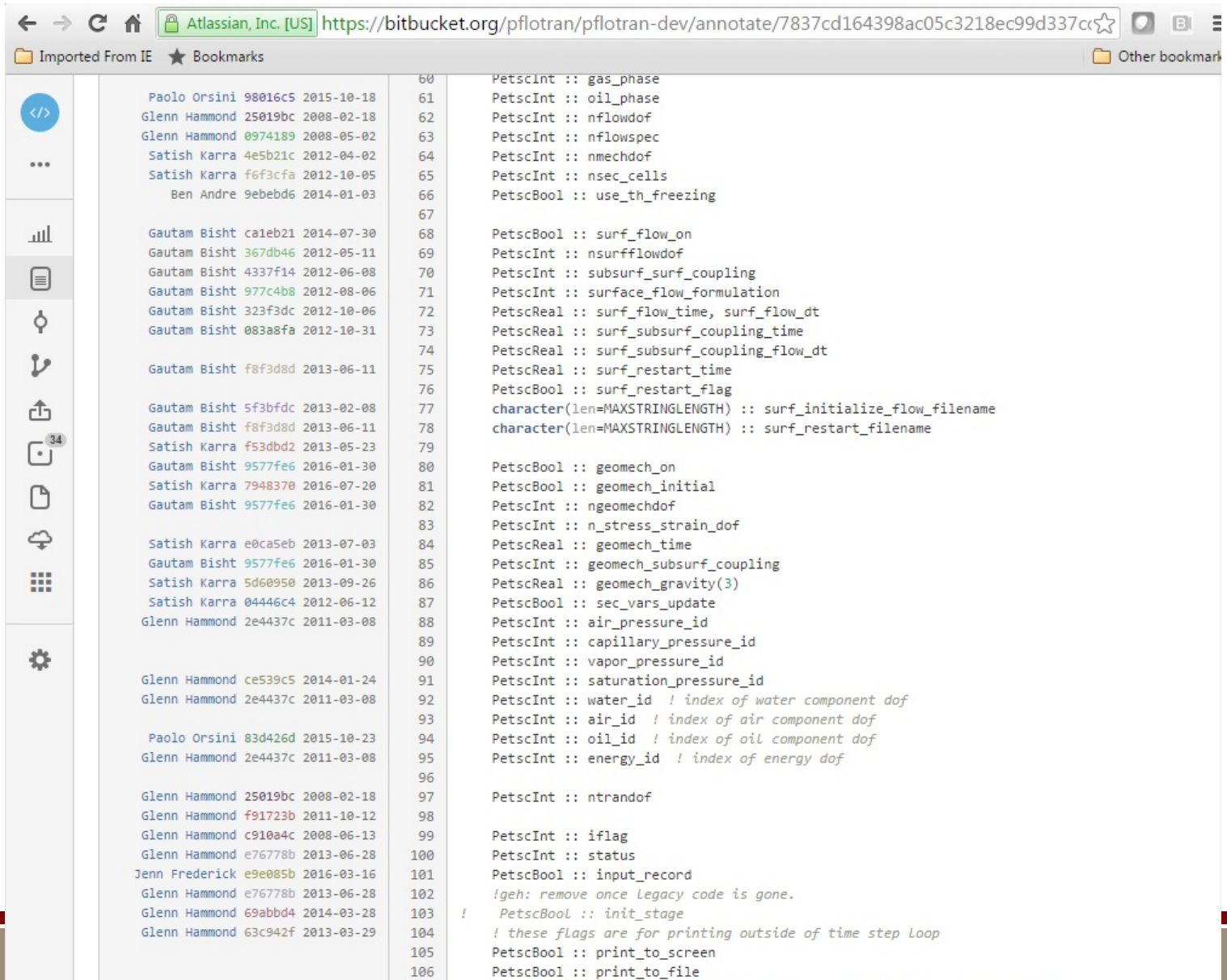
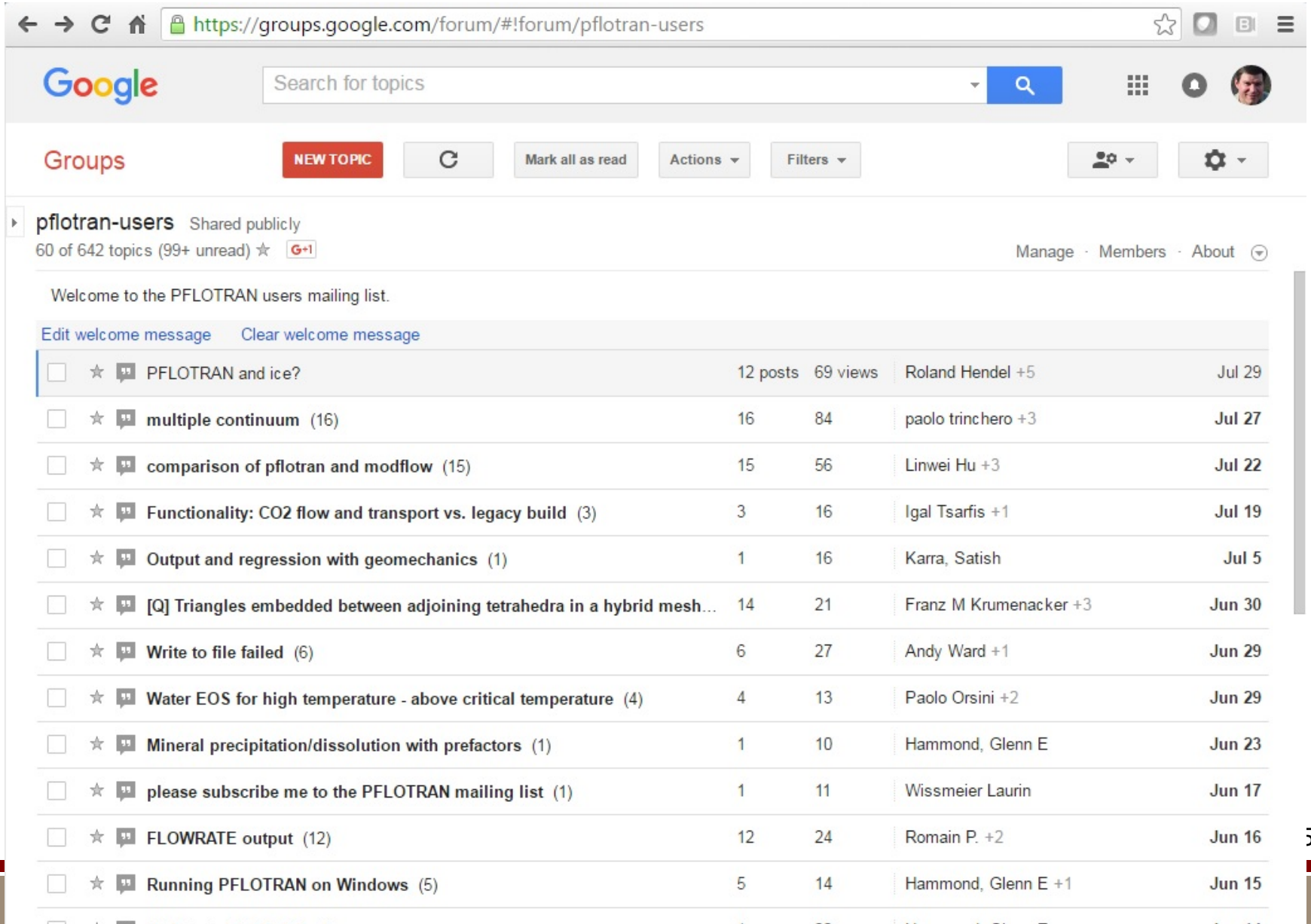


PFLOTRAN Bitbucket Blame



Paolo Orsini 98016c5 2015-10-18	60	PetscInt :: gas_phase
Glenn Hammond 25019bc 2008-02-18	61	PetscInt :: oil_phase
Glenn Hammond 0974189 2008-05-02	62	PetscInt :: nflowdof
Satish Karra 4e5b21c 2012-04-02	63	PetscInt :: nflowspec
Satish Karra f6f3cfa 2012-10-05	64	PetscInt :: nmechdof
Ben Andre 9ebebd6 2014-01-03	65	PetscInt :: nsec_cells
	66	PetscBool :: use_th_freezing
	67	
Gautam Bisht ca1eb21 2014-07-30	68	PetscBool :: surf_flow_on
Gautam Bisht 367db46 2012-05-11	69	PetscInt :: nsurfflowdof
Gautam Bisht 4337f14 2012-06-08	70	PetscInt :: subsurf_surf_coupling
Gautam Bisht 977c4b8 2012-08-06	71	PetscInt :: surface_flow_formulation
Gautam Bisht 323f3dc 2012-10-06	72	PetscReal :: surf_flow_time, surf_flow_dt
Gautam Bisht 083a8fa 2012-10-31	73	PetscReal :: surf_subsurf_coupling_time
	74	PetscReal :: surf_subsurf_coupling_flow_dt
Gautam Bisht f8f3d8d 2013-06-11	75	PetscReal :: surf_restart_time
	76	PetscBool :: surf_restart_flag
Gautam Bisht 5f3bfdc 2013-02-08	77	character(len=MAXSTRINGLENGTH) :: surf_initialize_flow_filename
Gautam Bisht f8f3d8d 2013-06-11	78	character(len=MAXSTRINGLENGTH) :: surf_restart_filename
Satish Karra f53dbd2 2013-05-23	79	
Gautam Bisht 9577fe6 2016-01-30	80	PetscBool :: geomech_on
Satish Karra 7948370 2016-07-20	81	PetscBool :: geomech_initial
Gautam Bisht 9577fe6 2016-01-30	82	PetscInt :: ngeomechdof
	83	PetscInt :: n_stress_strain_dof
Satish Karra e0ca5eb 2013-07-03	84	PetscReal :: geomech_time
Gautam Bisht 9577fe6 2016-01-30	85	PetscInt :: geomech_subsurf_coupling
Satish Karra 5d60950 2013-09-26	86	PetscReal :: geomech_gravity(3)
Satish Karra 04446c4 2012-06-12	87	PetscBool :: sec_vars_update
Glenn Hammond 2e4437c 2011-03-08	88	PetscInt :: air_pressure_id
	89	PetscInt :: capillary_pressure_id
	90	PetscInt :: vapor_pressure_id
Glenn Hammond ce539c5 2014-01-24	91	PetscInt :: saturation_pressure_id
Glenn Hammond 2e4437c 2011-03-08	92	PetscInt :: water_id ! index of water component dof
	93	PetscInt :: air_id ! index of air component dof
Paolo Orsini 83d426d 2015-10-23	94	PetscInt :: oil_id ! index of oil component dof
Glenn Hammond 2e4437c 2011-03-08	95	PetscInt :: energy_id ! index of energy dof
	96	
Glenn Hammond 25019bc 2008-02-18	97	PetscInt :: ntrandof
Glenn Hammond f91723b 2011-10-12	98	
Glenn Hammond c910a4c 2008-06-13	99	PetscInt :: iflag
Glenn Hammond e76778b 2013-06-28	100	PetscInt :: status
Jenn Frederick e9e085b 2016-03-16	101	PetscBool :: input_record
Glenn Hammond e76778b 2013-06-28	102	!geh: remove once legacy code is gone.
Glenn Hammond 69abbd4 2014-03-28	103	! PetscBool :: init_stage
Glenn Hammond 63c942f 2013-03-29	104	! these flags are for printing outside of time step loop
	105	PetscBool :: print_to_screen
	106	PetscBool :: print_to_file

PFLOTRAN User Support



Hits on PFLOTRAN Bitbucket Site in 2015

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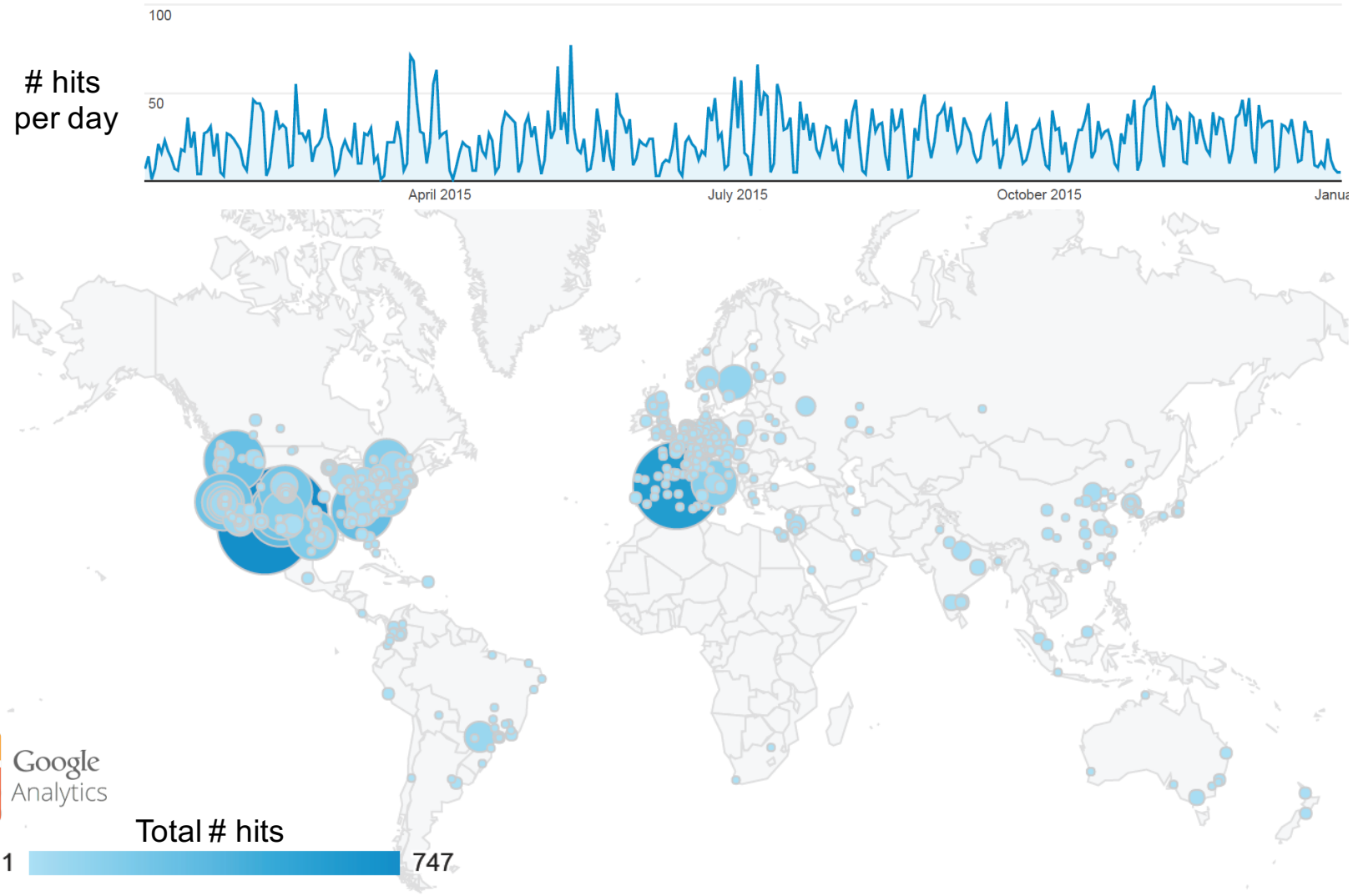
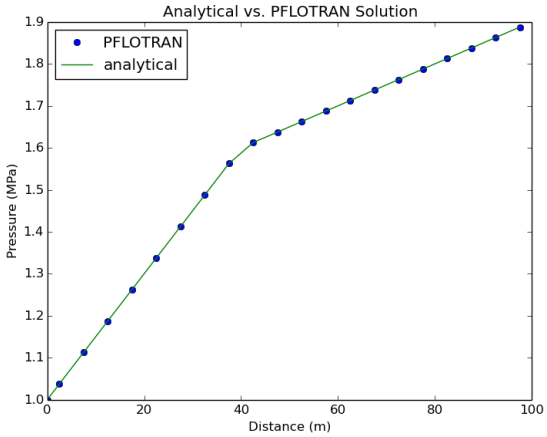
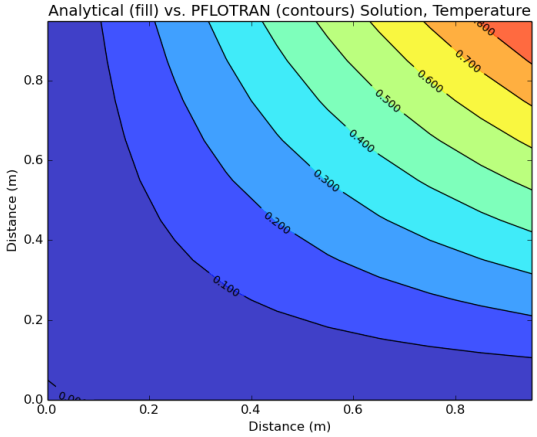
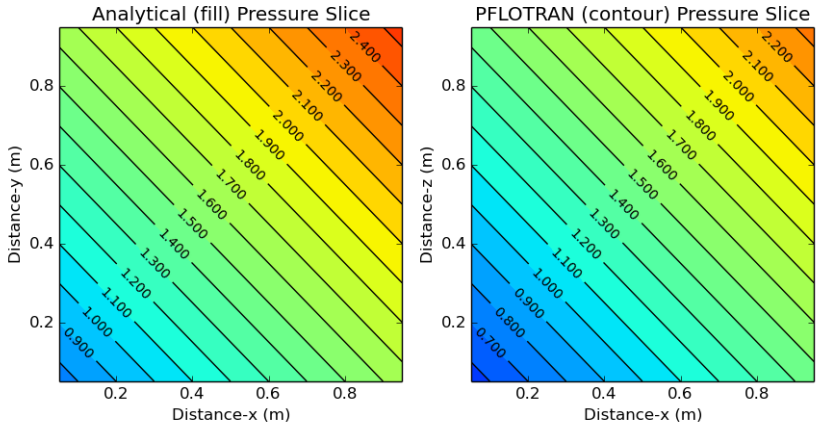


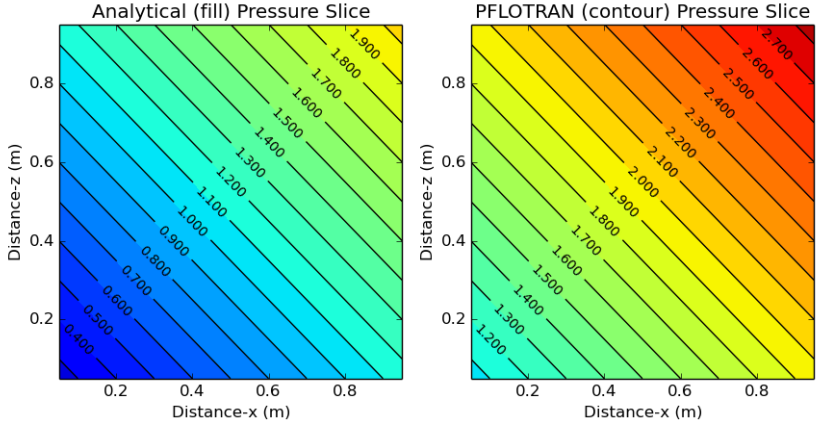
PFLOTRAN QA Testing

python-scripted framework under development





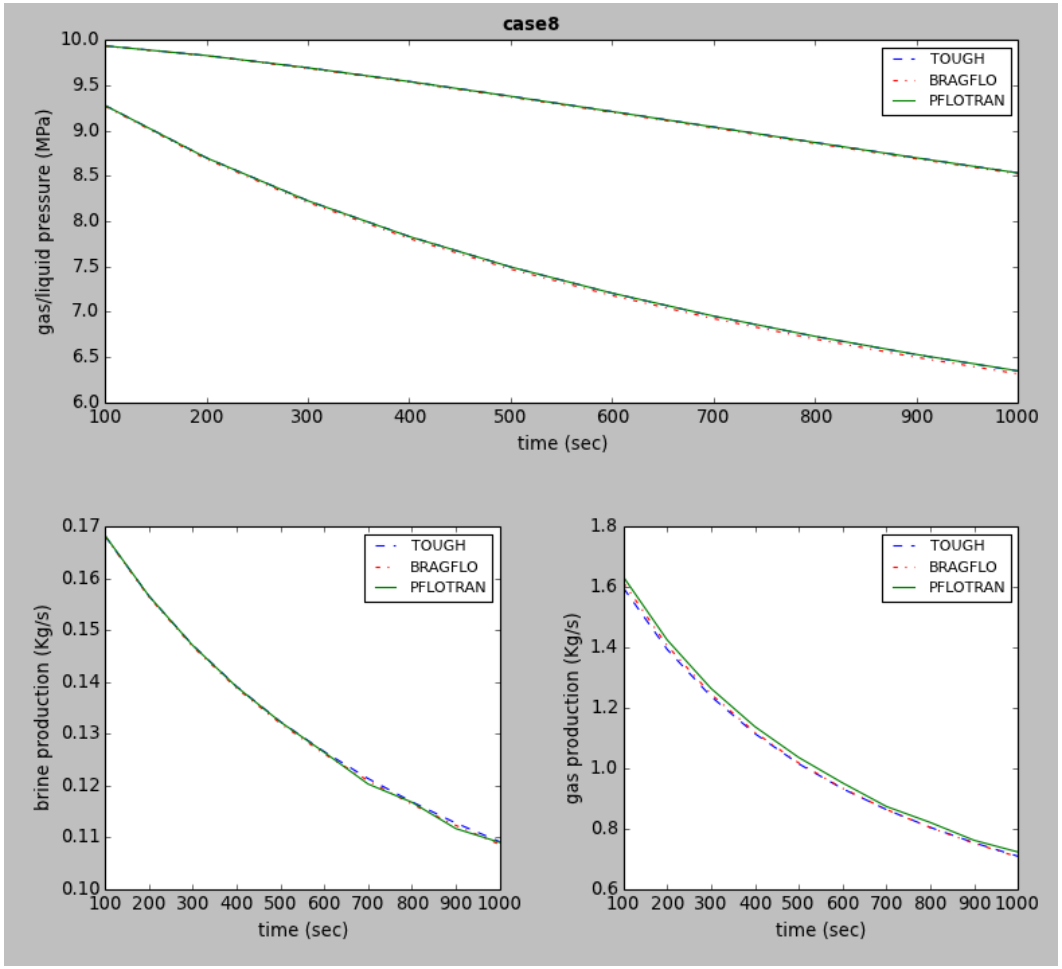




PFLOTRAN Verification Testing

- 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)



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QUESTIONS?

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MODERN FORTRAN

Why Object-Oriented Fortran 2003/2008?

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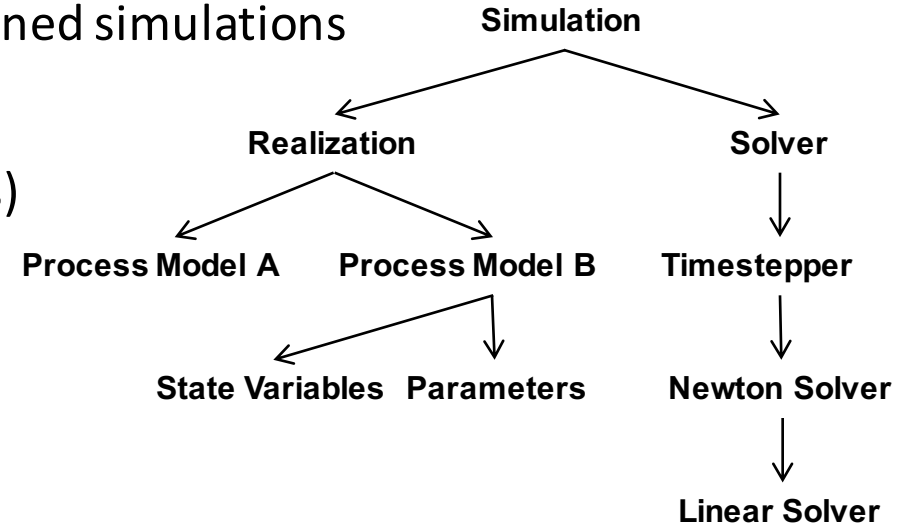
- Why Fortran?
  - Experienced domain scientists remain engaged
  - Commonality among all domain scientists
- Why object-oriented?
  - Modular data structures
    - Eases code development and debugging – data locality
    - Nesting of processes and data
  - Tree structure enables self-contained simulations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



Object-Oriented Fortran

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Fortran 77

```
subroutine X(a,b,c,d,e,f,…)

...

common/array/a(ncomp,ncell)



do icell = 1, ncell
  do icomp = 1, ncomp
    a(icomp,icell) = …
  enddo
enddo
```

OO Fortran 90

```
subroutine X(realization)

...

grid => realization%patch%grid
reaction => realization%reaction
cells => realization%patch…%cells

do icell = 1, grid%ncell
  do icomp = 1, reaction%ncomp
    cells(icell)%conc(icomp) = …
  enddo
enddo
```

Modern Fortran

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Fortran 90

```
select case(eos_type)
  case(WATER)
    call EvaluateWater(p,t)
  case(AIR)
    call EvaluateAir(p,t)
  case(CO2)
    call EvaluateCO2(p,t)
  case(CH4)
    call EvaluateCH4(p,t)
end select
```

Fortran 2003/2008

```
type, extends(eos_base) :: eos_CO2
  …
contains
  procedure :: Evaluate => EvaluateCO2
end type eos_CO2

class(eos_CO2) :: eos

call eos%Evaluate(p,t)
```

eos = equation of state