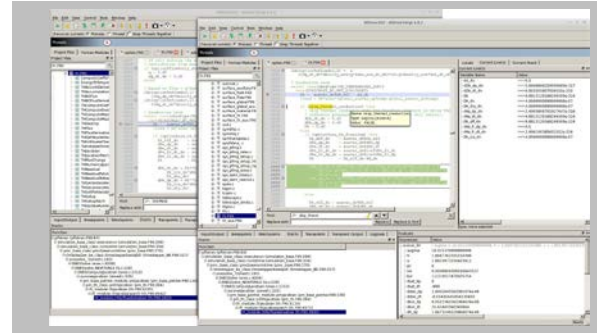


*Exceptional service in the national interest*

```
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.
```

last build	dev-std-gnu-linux	dev-std-gnu-mac	
	build successful	build successful	
current activity	waiting next in ~ 9 hrs 40 mins at 01:00	waiting next in ~ 9 hrs 40 mins at 01:00	
PDT	changes	dev-std-gnu-linux	dev-std-gnu-mac
01:12:50			
01:12:00			
01:04:54		test pflotran studio	test pflotran studio
01:04:36		build pflotran studio	build pflotran studio
		petsc studio	petsc studio
		set build script path	set build script path
		property 'pflotran_dir' set studio property changes	property 'pflotran_dir' set studio property changes



# PFLOTRAN Testing

# Testing

- 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.)

- 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.)

- 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/unittests'
-----
Running pflotran unit tests :
.....
Time:          0.001 seconds

OK
(38 tests)
-----
make[1]: Leaving directory `/home/gehammo/software/pflotran-dev/src/pflotran/unittests'
make[1]: Entering directory `/home/gehammo/software/pflotran-dev/regression_tests'
/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-calcite
-----
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| > tolerance:+0.1000000E-15.

FAILURES!!!
Tests run: 38, Failures: 1, Errors: 0
-----
make[1]: Leaving directory `/home/gehammo/software/pflotran-dev/src/pflotran/unittests'
make[1]: Entering directory `/home/gehammo/software/pflotran-dev/regression_tests'
/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-calcite
-----
Test log file : pflotran-tests-2016-07-29_10-27-50.testlog
Running pflotran regression tests :
.....F.F....FFFFFF..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

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.
```

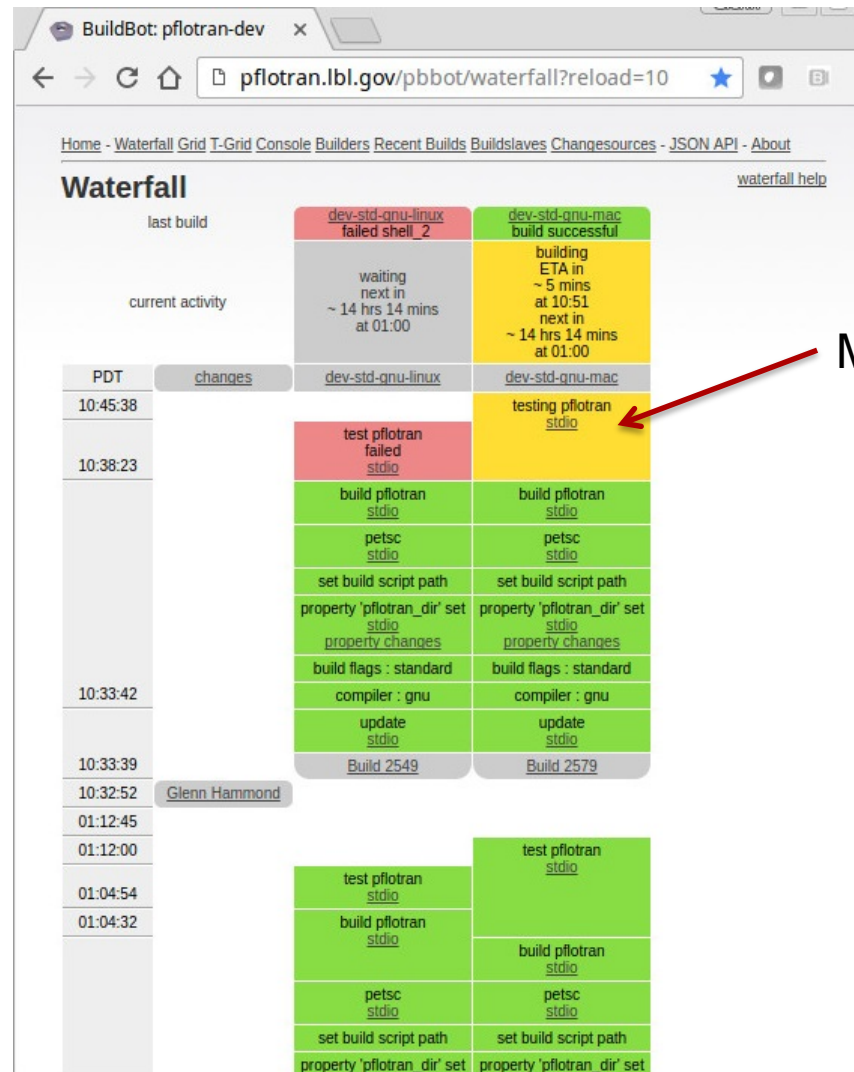
```
-----  
543_hanford_srfcplx_param...  
  cd /home/gehammo/software/pflotran-dev/regression_tests/default/543  
  /home/gehammo/software/pflotran-dev/src/pflotran/pflotran -malloc 0 -successful_exit_code 86 -input_prefix  
543_hanford_srfcplx_param  
  # 543_hanford_srfcplx_param : run time : 2.91 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: UO2S04 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.
```

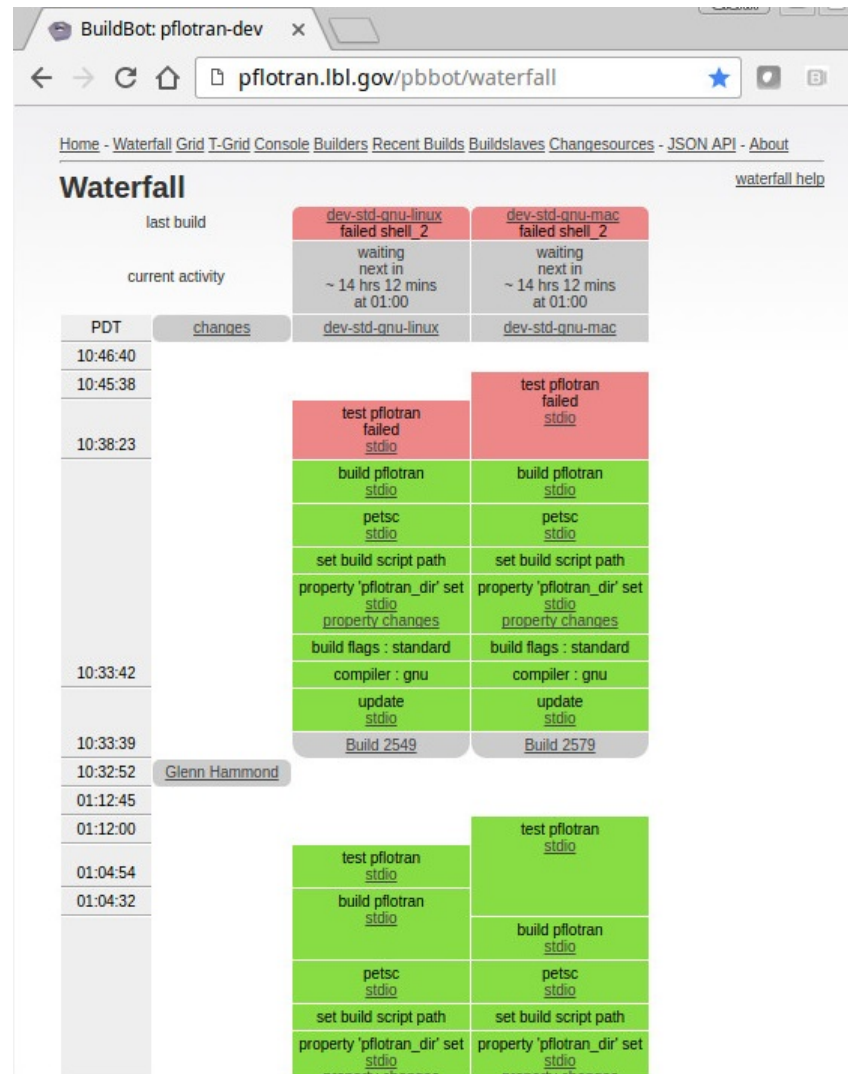
```
-----  
543_hanford_srfcplx_param...  
  cd /home/gehammo/software/pflotran-dev/regression_tests/default/543  
  /home/gehammo/software/pflotran-dev/src/pflotran/pflotran -malloc 0 -successful_exit_code 86 -input_prefix  
543_hanford_srfcplx_param  
  # 543_hanford_srfcplx_param : run time : 2.91 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: UO2S04 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



The screenshot shows a web browser window with the URL `pflotran.lbl.gov/pbbot/waterfall`. The page title is "Waterfall" and it includes navigation links for "Home", "Waterfall", "Grid", "T-Grid", "Console", "Builders", "Recent Builds", "Buildslaves", "Changesources", "JSON API", and "About". A "waterfall help" link is also present.

The main content is a waterfall chart with two columns representing different build environments: `dev-std-gnu-linux` and `dev-std-gnu-mac`. The chart shows the following sequence of jobs:

- last build:** `dev-std-gnu-linux` failed shell\_2; `dev-std-gnu-mac` failed shell\_2.
- current activity:** Both environments are "waiting next in ~ 14 hrs 12 mins at 01:00".
- changes:** A "changes" event is shown in the PDT column.
- Build 2549 (dev-std-gnu-linux):** A sequence of jobs including "update stdio", "compiler : gnu", "build flags : standard", "property 'pflotran\_dir' set stdio", "set build script path", "petsc stdio", and "build pflotran stdio".
- Build 2579 (dev-std-gnu-mac):** A sequence of jobs including "update stdio", "compiler : gnu", "build flags : standard", "property 'pflotran\_dir' set stdio", "set build script path", "petsc stdio", and "build pflotran stdio".
- test jobs:** "test pflotran stdio" jobs are shown for both environments, with the mac version failing.

A user "Glenn Hammond" is shown in the PDT column at 10:32:52.