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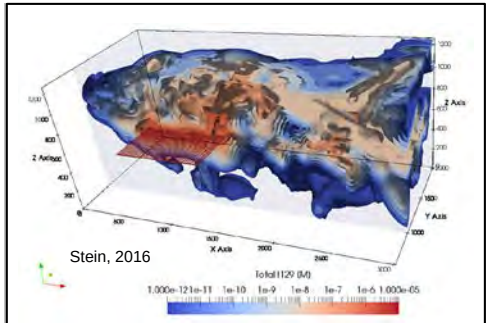
soft·ware ev·o·lu·tion
ˈsôf(t)wer/ /ˌevəˈlo͞oSH(ə)n/

Standard definition:

The gradual development of code, from a simple to a more complex form, due to ***repeated*** improvements and updates.



git

LGPL Free Software
Free as in Freedom

PFLOTRAN

Atlassian Bitbucket

Maintaining Quality Assurance Within Software Evolution: Lessons Learned With PFLOTRAN

Jennifer M. Frederick and Glenn E. Hammond

SAND2017-9211-C

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

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What is Software Evolution?

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soft·ware ev·o·lu·tion

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New domain science:

- New process models
- Increasingly mechanistic process models
- Programming paradigms
- Novel numerical methods

What is Software Evolution?

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soft·ware ev·o·lu·tion

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New computational science:

- Changing third party libraries
- Changing operating systems
- Changing programming language
- New or architecturally changing computer hardware

What is Software Evolution?

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soft·ware ev·o·lu·tion

ˈsôf(t)wer/ /ˌevəˈlo͞oSH(ə)n/

Standard definition:

> The gradual development of code, from a simple to a more complex form, due to ***repeated*** improvements and updates.

When software is constantly evolving, how can we ensure software quality?

What is Software Quality Assurance?

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soft·ware qual·i·ty as·sur·ance

ˈsôf(t)wer/ ˈkwäləd̄ē/ əˈSHo͝orəns/

IEEE standard:

> A planned and systematic pattern of all actions necessary **to provide adequate confidence** that software conforms to established technical requirements.

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Software quality includes:

- **Correctness**
- **Reliability**
- Efficiency
- Survivability
- **Maintainability**
- **Testability**
- **Availability**
- Portability

What is Software Quality Assurance?

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soft·ware qual·i·ty as·sur·ance

ˈsôf(t)wer/ ˈkwäləd ē/ əˈSHo o r ə n s/

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How does PFLOTRAN ensure software quality under an evolving software framework?

PFLOTRAN

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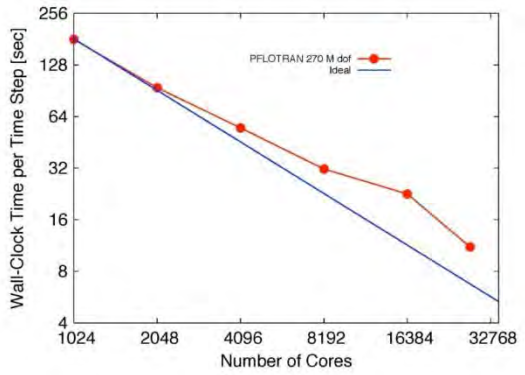
www.pflotran.org

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



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

PFLOTRAN

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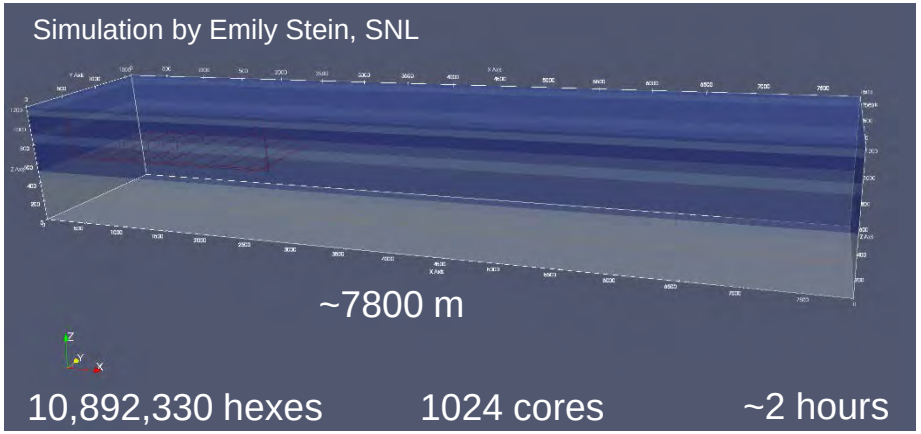
- Nuclear waste disposal
  - Waste Isolation Pilot Plant (WIPP) in Carlsbad, NM
  - DOE Spent Fuel and Waste Science & Technology Program
  - SKB Forsmark Spent Fuel Nuclear Waste Repository (Sweden, Amphos^{21})
- Climate: coupled overland/groundwater flow; CLM
  - Next Generation Ecosystem Experiments (NGEE) Arctic
  - DOE Earth System Modeling (ESM) Program
- Biogeochemical transport modeling
- CO_2 sequestration
- Enhanced geothermal energy
- Radioisotope tracers
- Colloid-facilitated transport

pa.sandia.gov



Steps taken to minimize impacts of software evolution:

- Open source development
- Software configuration management
- Modular object oriented design
- Automated testing suites
- Online documentation

Open Source Development

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- Google

  "Open source is an adjective denoting software for which the original source code is made freely available and may be redistributed and modified."

- Open source software refers to code that:
  - Is free
  - Is publicly available
  - Can be legally modified
  - Can be legally shared with anyone

Open Source Development

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- PFLOTRAN has an open source GNU Lesser General Public License (LGPL).
  - The original or modified source may not be sold for profit.
  - Third-party software linked to or wrapped around PFLOTRAN (e.g. graphical user interfaces [GUIs], pre-/post-processing tools, etc.) may be proprietary.

Benefits of Open Source Software

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- Encourages collaboration
  - Development, testing, debugging can be shared

critical for software quality assurance

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

Software Configuration Management

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- PFLOTRAN employs the Git distributed source control management tool for configuration management.
- Git logs all changes to a code repository
  - version control
- Git allows developers to:
  - Clone the base repository
  - Modify and test code in a development branch
  - Merge changes back into base repository
  - Pinpoint problematic changesets (snapshots of code versions)

critical for software quality assurance

Software Configuration Management

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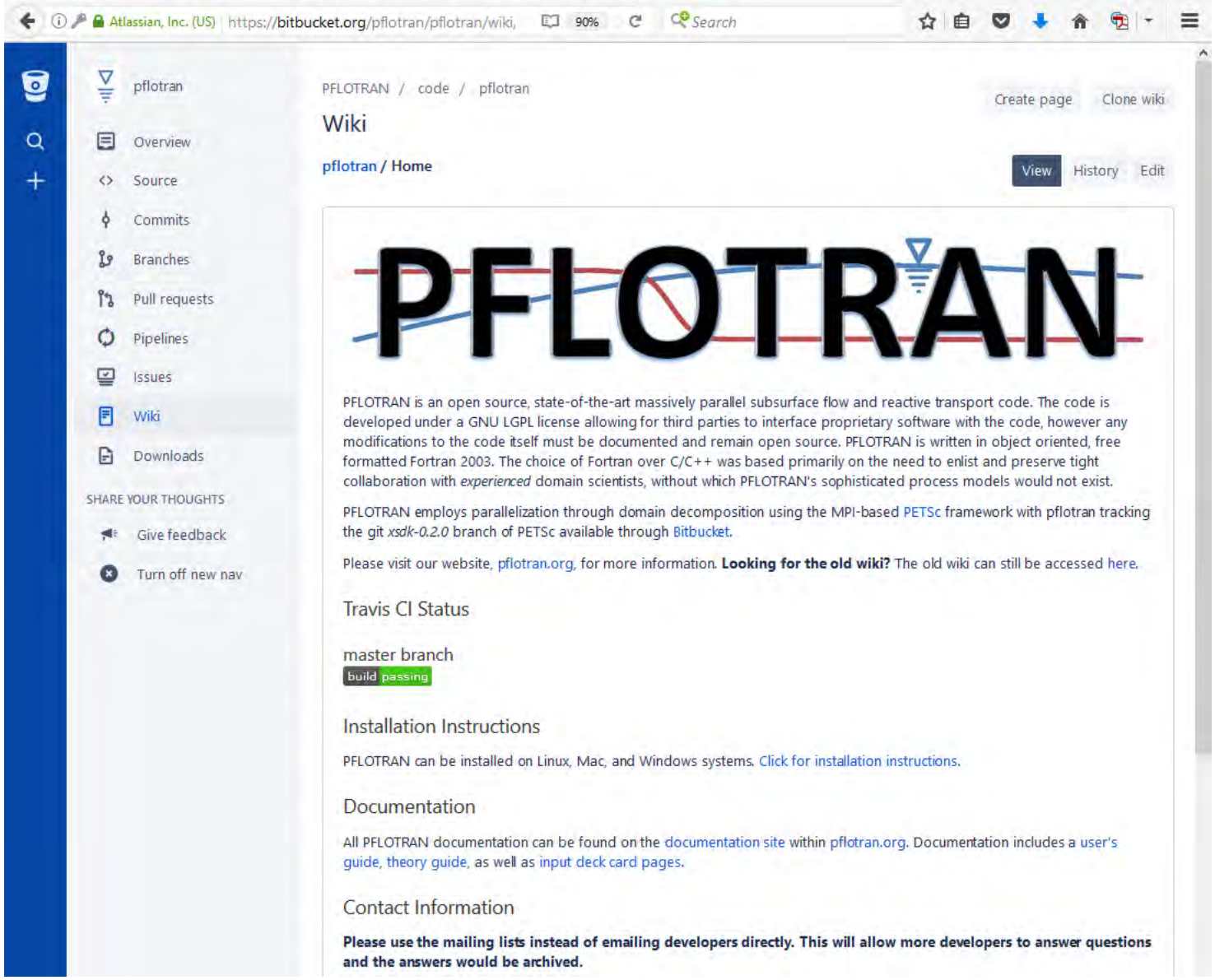
- The PFLOTRAN source code repository is hosted at Bitbucket.org.

  https://bitbucket.org/pflotran/pflotran

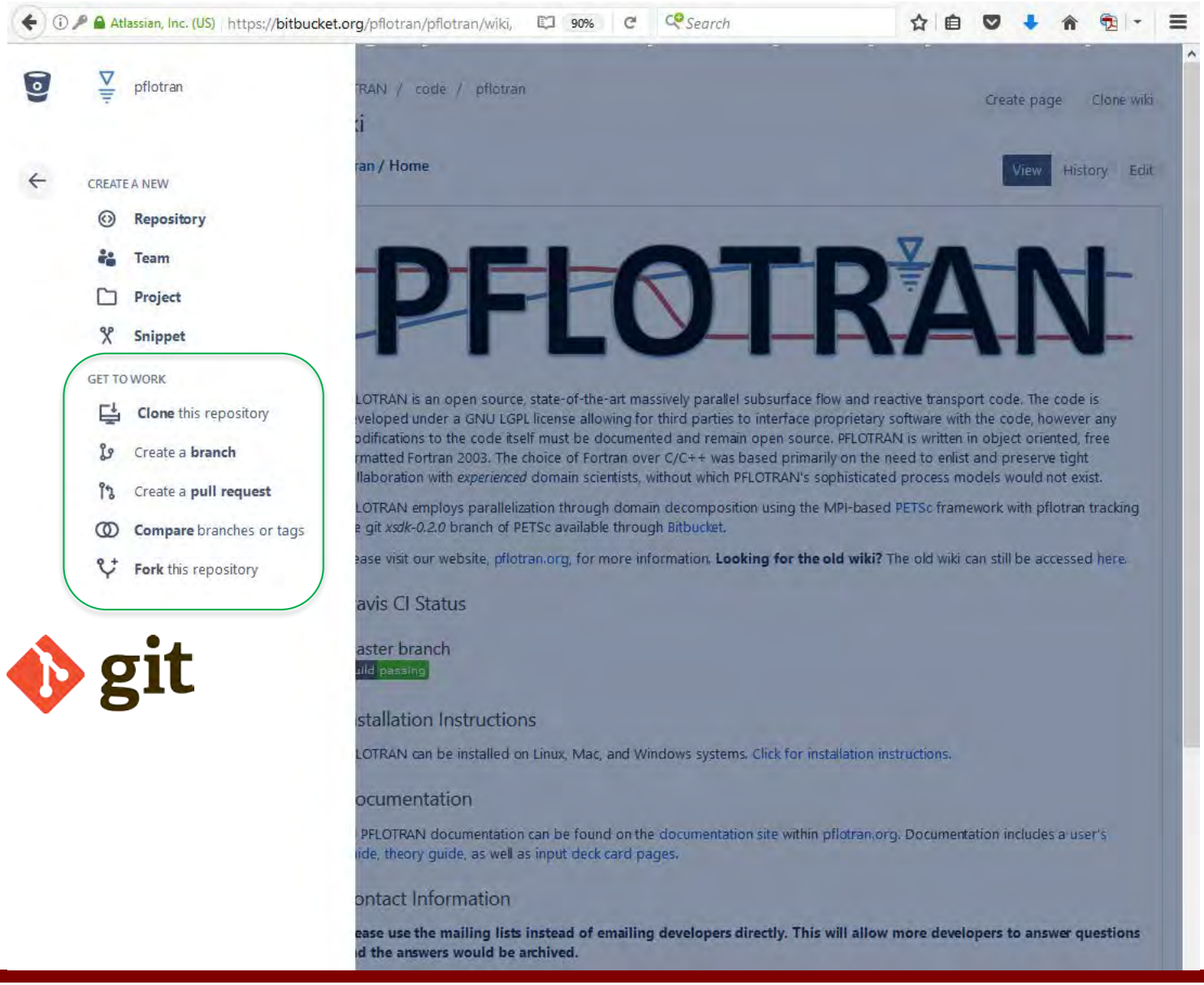
critical for software quality assurance (availability)

- Bitbucket is a web-based hosting service for software development projects that use Git.
- Provides:
  - Git operations (clone, fork, branch, etc.)
  - Wiki for information or documentation
  - Source tree
  - Pull requests
  - Commit logs
  - Issue tracker

Software Configuration Management



Software Configuration Management



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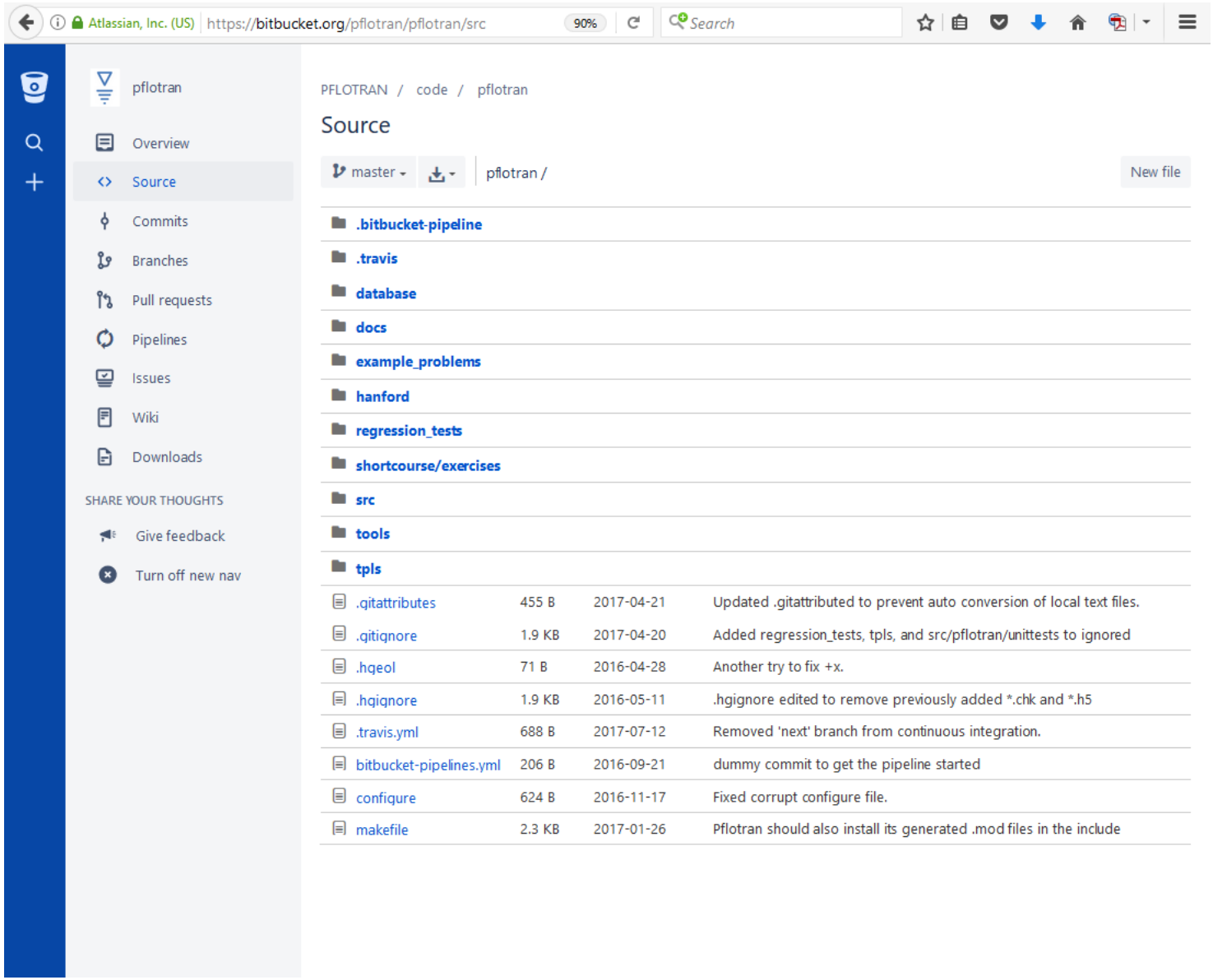
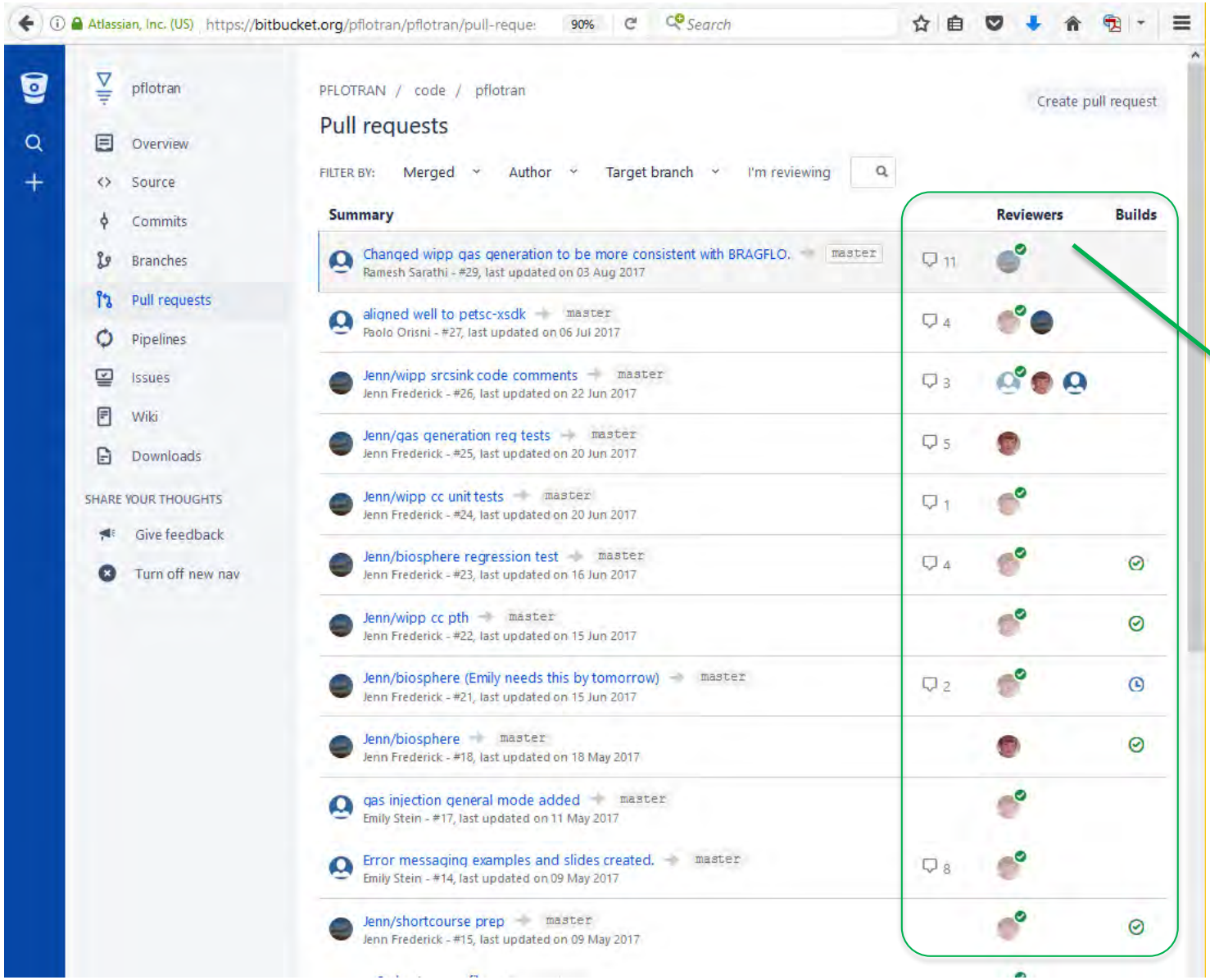


Software Configuration Management



Pull requests are reviewed, commented on, and scrutinized by a second pair of eyes.

Software Configuration Management

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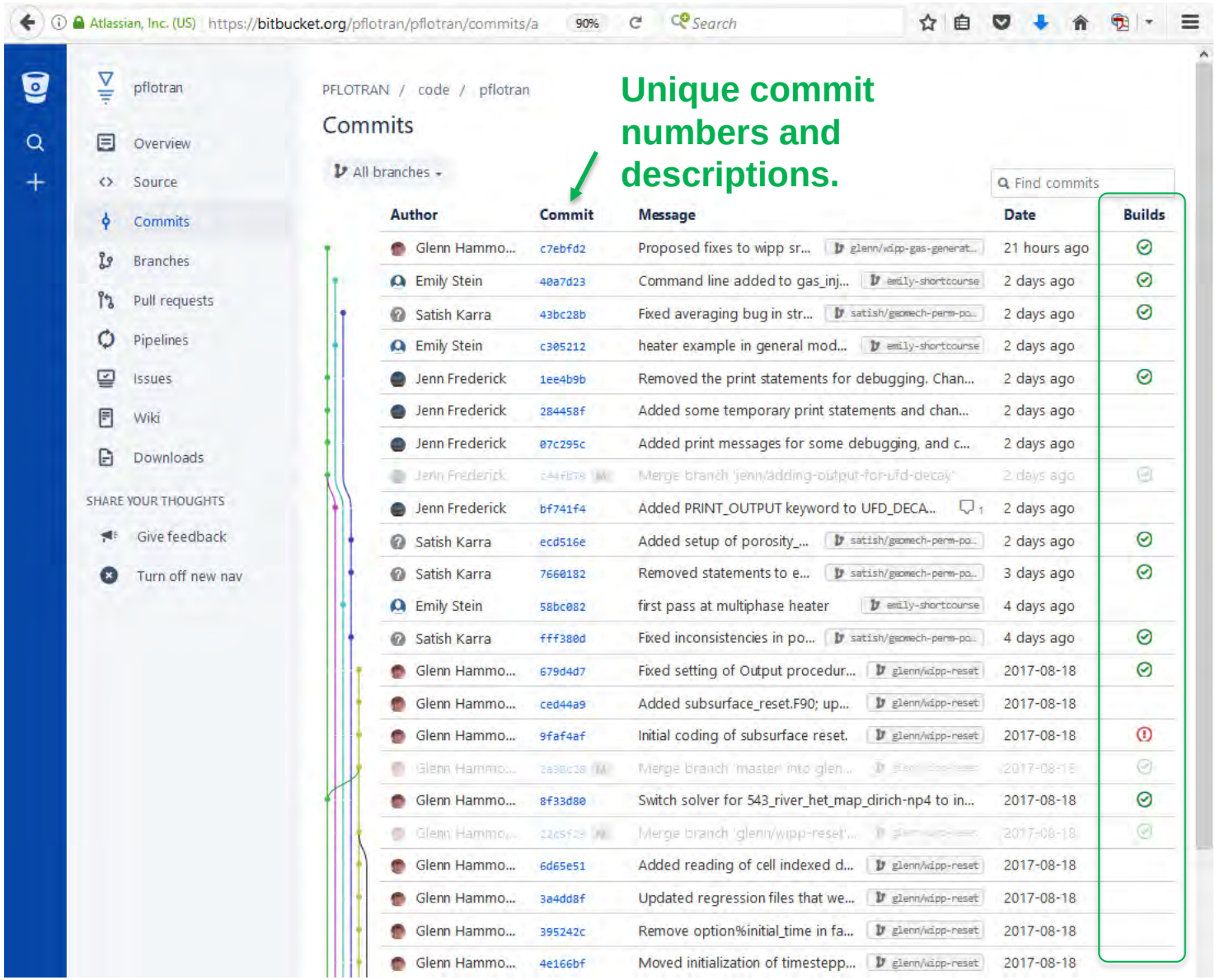

Automatic builds each time the code has changed.

Modular Object Oriented Design

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- Object oriented design involves the organization of data and procedures into a hierarchy of containers (objects).
- The use of objects:
  - Improves data locality (modularity)
  - Eases code refactoring (rewriting)
  - Facilitates extensibility (for adding capability)

critical for software quality assurance (maintainability)

- PFLOTRAN uses object oriented modern **FORTRAN 2003/2008**

Automated Testing Suites

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- As open source development fosters a growing community of developers, the code can't break!.
- **Unit tests**
  - Individual routines are executed in isolation.
  - Results are compared with a gold standard to *within a tolerance*.
- **Regression tests** – focus on changes in simulation results
  - Full simulations are executed.
  - Simulations results are sampled and compared to a gold standard to *within a tolerance*.
- **Verification tests**
  - Full simulations are executed, for which there is a known solution.
  - Simulation results are sampled and compared to an analytical solution *within a tolerance*.

```
if (abs(test_value – gold_standard) > tolerance) report_error()
```

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Why a tolerance?
Accommodates small variations in software and hardware configurations (Linux vs Mac)

```
if (abs(test_value – gold_standard) > tolerance) report_error()
```

Automated Testing Suites: Regression Tests

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This is what a successful run of the unit tests and regression tests looks like:

```
[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
 (36 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.
```

Automated Testing Suites: Regression Tests

- Example regression test failure:
  - Perturb the critical pressure for the 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
```

Automated Testing Suites: Regression Tests

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This is what a failed run of the unit tests and regression tests looks like:

```
------------------------------------------------------------------------
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
```

Automated Testing Suites: Regression Tests

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.
```

this test didn't use the change in eos_water.f90, so it passes

this test used the change in eos_water.f90, so it fails

Automated Testing Suites: Verification Tests

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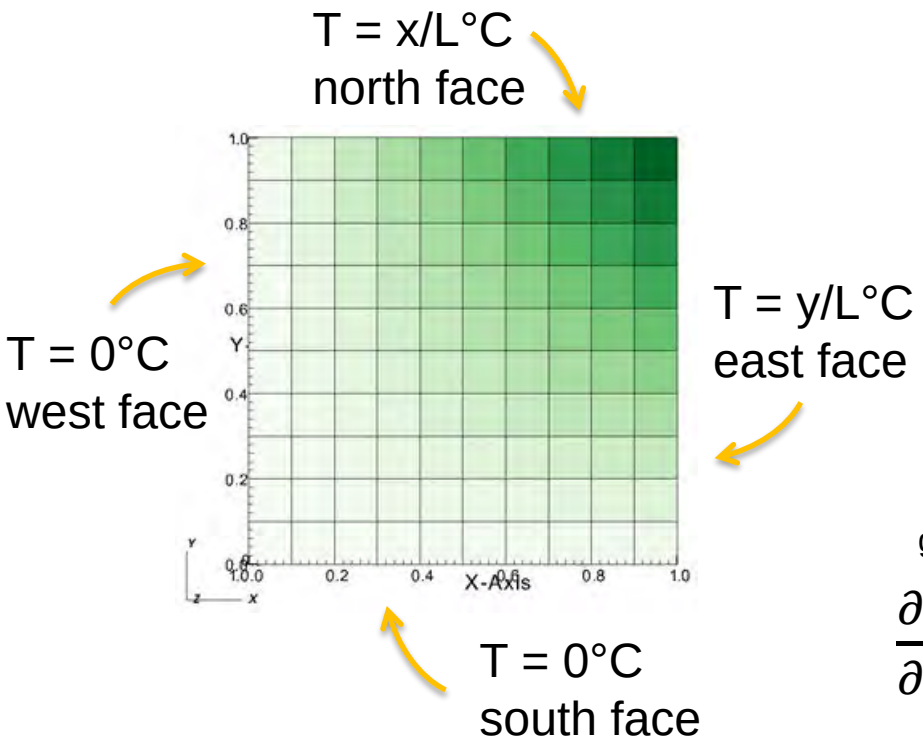
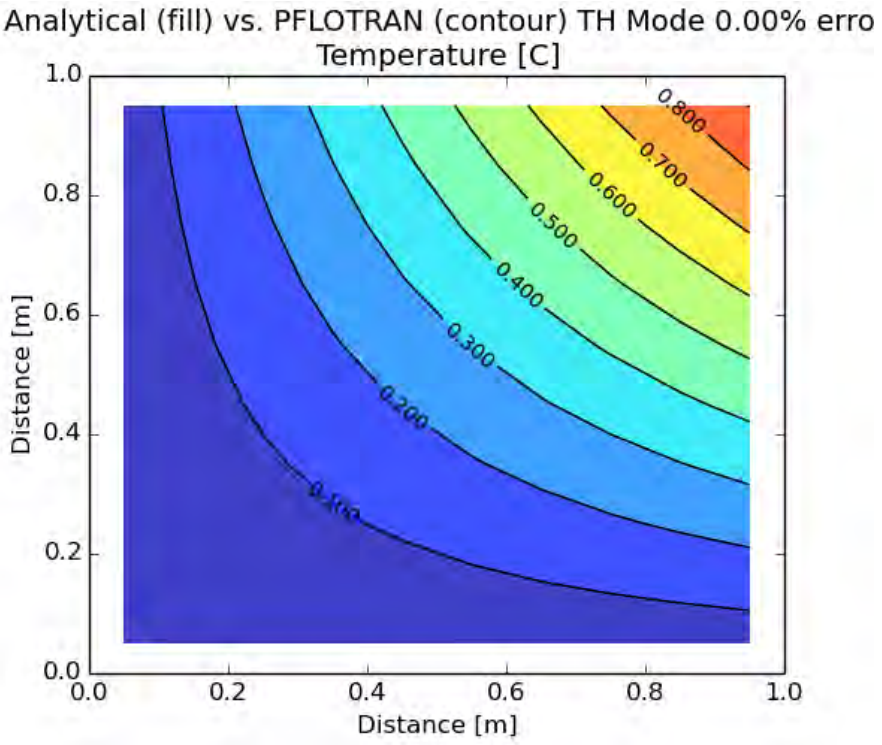
- A set of > 50 tests that verify the code against an analytical solution
- Automatic spatial convergence testing is also performed
- The tests can be run each time a major portion of the code changes

```
==========================================
  3D, Steady, Thermal, BCs 1st kind, TH Mode
==========================================
Running PFLOTRAN simulation . . .
Relative Maximum Error:  1.07799999995 %
-- Test PASS --


================================================================
====== Running STEADY THERMAL tests ============================
================================================================
====== GENERAL Mode ============================================
================================================================
/home/jmfrede/software/pflotran-qa/qa_tests/thermal/steady

==================================================
  1D, Steady, Thermal, BCs 1st kind, General Mode
==================================================
Running PFLOTRAN simulation . . .
Relative Maximum Error:  0.0 %
-- Test PASS --

==========================================================
  1D, Steady, Thermal, BCs 1st/2nd kind, General Mode
==========================================================
Running PFLOTRAN simulation . . .
Relative Maximum Error:  1.32563943235e-14 %
-- Test PASS --

==================================================
  2D, Steady, Thermal, BCs 1st kind, General Mode
==================================================
Running PFLOTRAN simulation . . .
Relative Maximum Error:  2.74129141815e-14 %
-- Test PASS --

==========================================================
  2D, Steady, Thermal, BCs 1st/2nd kind, General Mode
==========================================================
Running PFLOTRAN simulation . . .
Relative Maximum Error:  99.9999999333 %
-- Test FAIL --

==================================================
  3D, Steady, Thermal, BCs 1st kind, General Mode
==================================================
Running PFLOTRAN simulation . . .
Relative Maximum Error:  2.40048221534e-14 %
-- Test PASS --
```

Automated Testing Suites: Verification Tests

- 2D Domain (10x10 cells)
- Heat Conduction (steady state solution)
- Dirichlet (scalar) temperature boundary conditions





governing equation

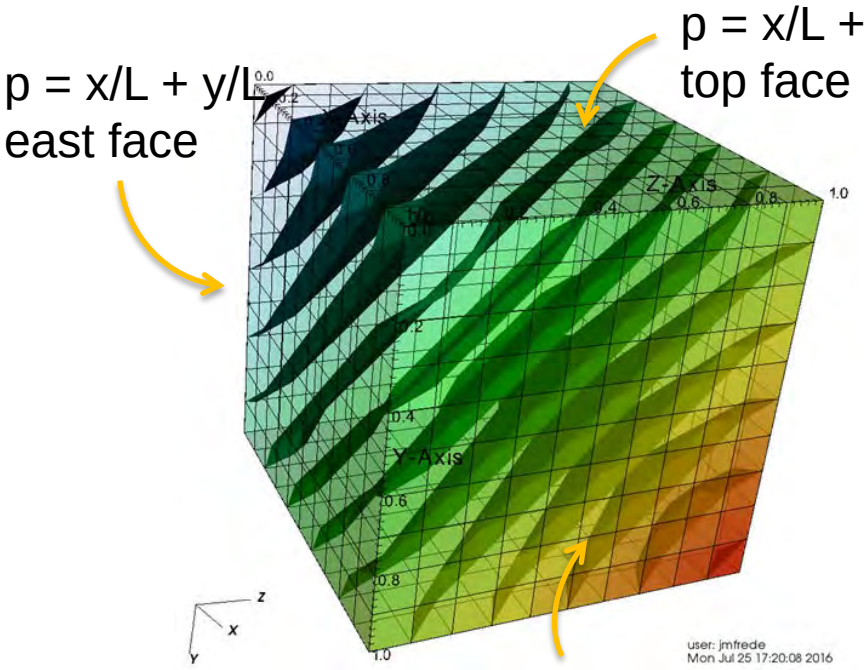
$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

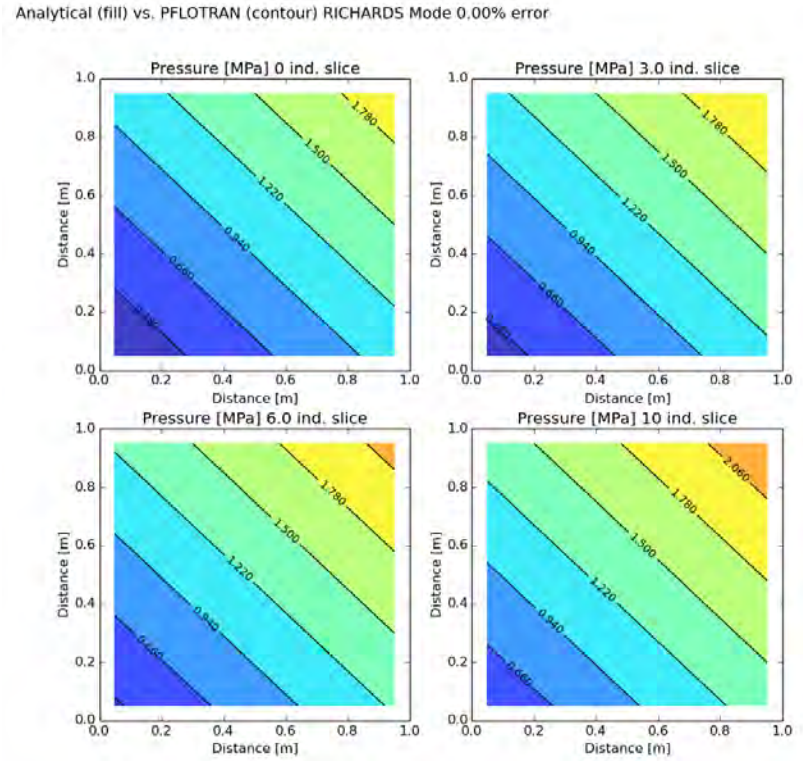
analytical solution

$$T(x,y) = T_0 \frac{x}{L} \frac{y}{L}$$

Automated Testing Suites: Verification Tests

- 3D Domain (10x10x10 cells)
- Fluid flow/pressure field (steady state solution)
- Dirichlet (scalar) pressure boundary conditions





governing equation

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + \frac{\partial^2 p}{\partial z^2} = 0$$

analytical solution

$$p(x, y, z) = p_0 \left(\frac{x}{L} + \frac{y}{L} + \frac{z}{L} \right)$$

PFLOTRAN's Online Documentation

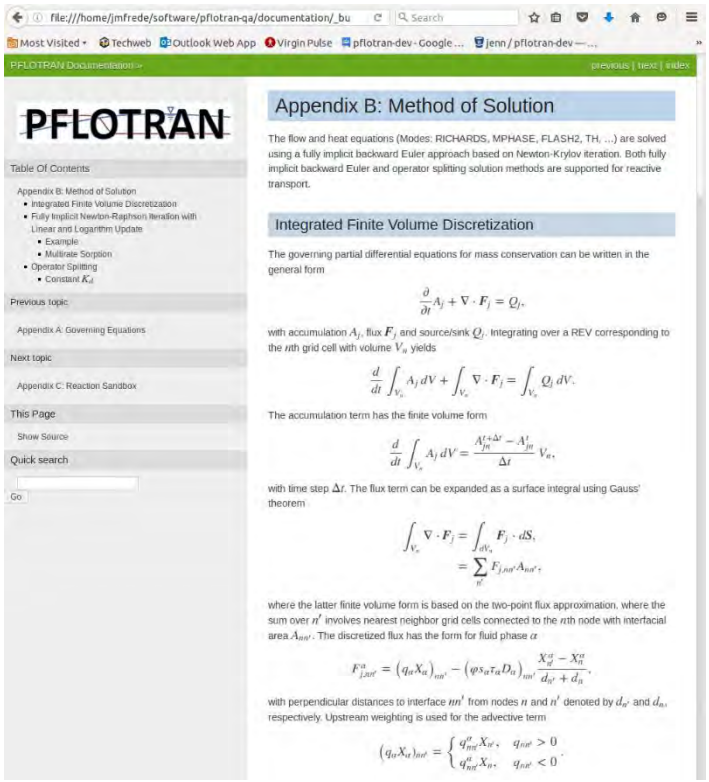
Sandia National Laboratories

Documentation pages are version controlled and also hosted on Bitbucket.org

documentation.pflotran.org

- We use a documentation generator program (Sphinx) to generate both the website and the PDF versions of the documentation:

SPHINX
Python Documentation Generator



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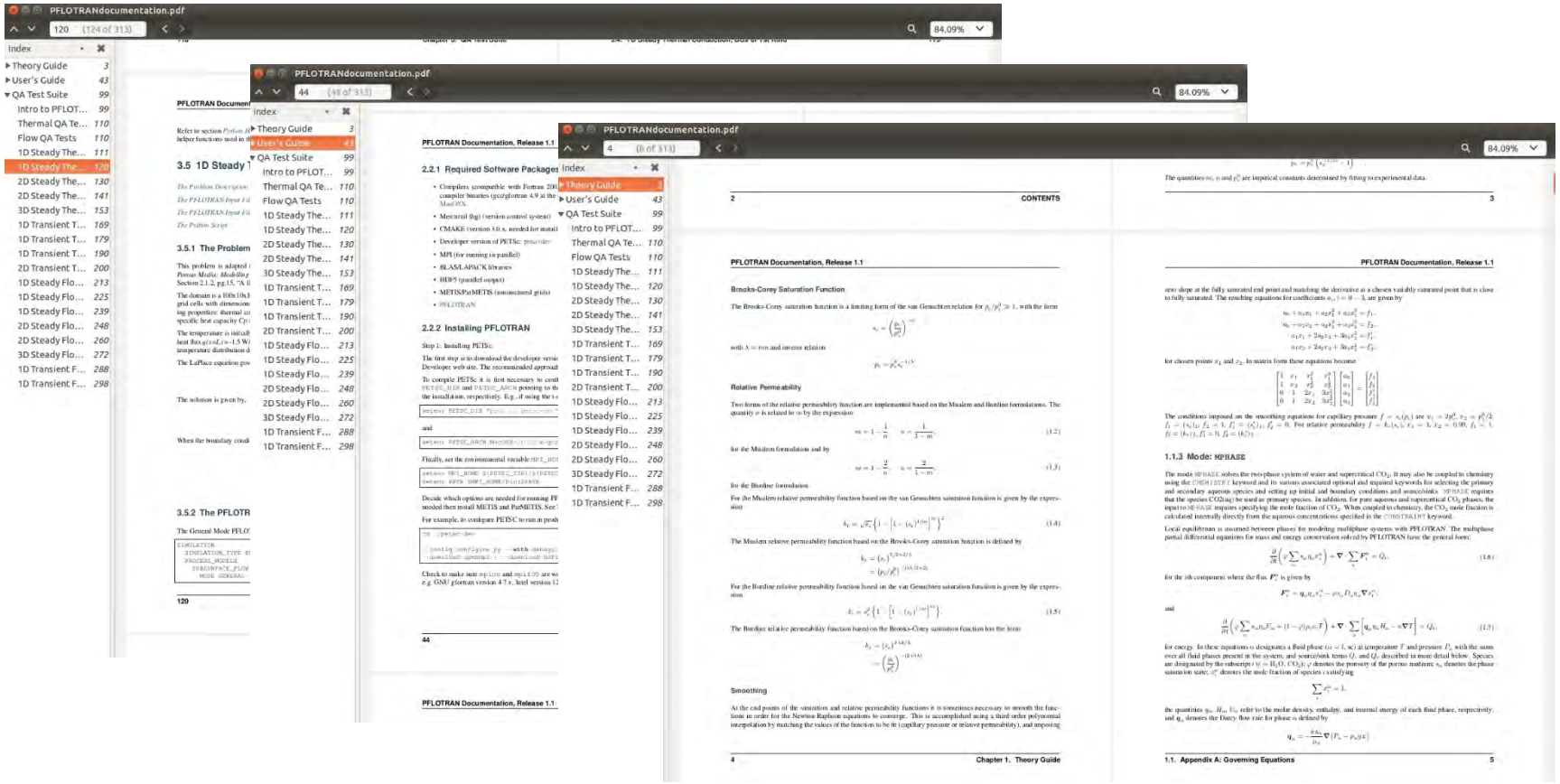

Conclusion

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- Although software tends to have a limited lifespan, careful design and planning in the development of a code can significantly lengthen the duration of a software application's viable existence.
- PFLOTRAN attempts to minimize the impact of software evolution through:
  - Open source development
  - Software configuration management
  - Modular object oriented design
  - Automated testing
  - Online documentation