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

**Open Source Development**
- Community contributions can drive the code to evolve beyond original vision
- More optimal use of funding
- Transparency exposes implementation details critical to scientific reproducibility, often excluded by scientific journals
- Encourages collaboration
- Benefits of Open Source Software
  - PFLOTRAN may be proprietary
  - The original or modified source code may not be sold for profit
  - Funding can be pooled across diverse sets of projects/budgets
  - Third-party software linked or wrapped around PFLOTRAN may be proprietary

**Maintaining Quality and Confidence in Open-Source, Evolving Software: Lessons Learned with PFLOTRAN**

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Software Configuration Management

- PFLOTRAN employs the Git distributed source control management tool for configuration management.
- Git tags all changes to a code repository
- Version control
- Code can be rolled back if a mistake was made
- 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)

Online Documentation

- PFLOTRAN uses a documentation generator program called Sphinx (www.sphinx-doc.org)
- The documentation consists of text files and images, written in restructured text, and organized with an index
- The documentation is version controlled and the repository is hosted on Bitbucket.com
- When/if you roll back the code, you can roll back the documentation tool!
- sphinx creates html files as well as Latex -> pdf
- We host the html files on our documentation website http://documentation.pflotran.org
- The pdf User’s Guide and Theory Manual can be downloaded or printed, and never falls behind the online documentation
- http://www.sphinx-docs.org

Automated Testing Suites

- Verification tests
  - Full simulations are executed, for which there is a known solution
  - Simulation results are sampled and compared to 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.
- Why a tolerance? Accommodates small variations in software and hardware (e.g., Linux vs Mac, compilers)

Example verification test failure:

```plaintext
+  pc1 = pc1 + 1.d-10*H2O_CRITICAL_PRESSURE
vc1 = 0.00317d0  ! m^3/kg
utc1 = one/tc1   ! 1/C
```

Example regression test failure:

```plaintext
--- a/src/pflotran/eos_water.F90
+  pc1 = pc1 + 1.d-10*H2O_CRITICAL_PRESSURE
```

A successful run of the unit and regression tests.

A successful run of the unit and regression tests.