Testing Fortran Software with pFunit

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Outline

- Unit Testing and Testing Frameworks
- Break for questions and discussion
- pFUnit – capabilities and examples
- Break for questions and discussion
- Obstacles to testing technical software and suggested remedies
Plato’s Cave (objective reality?)

Theory and Data

Mathematical Model

Discretization & Approximation

Implementation

Executable

Software Verification

Compiler Verification

Have we built the software right?

Verification and Validation

Have we built the right software?
Not all tests are created equal

➢ Abort?:
   if (x < 0.0) ERROR STOP “ILLEGAL VALUE FOR X”

➢ Diagnostic print statement:
   print*, ”loss of mass = ” , deltaMass

➢ Visual inspection / acceptance threshold for regression:
Anatomy of a Unit Test

\[ x(t) = x_0 + v_0(t-t_0) + \frac{1}{2} a (t-t_0)^2 \]

- **set preconditions**
- **invoke system-under-test**

**check #1**

**FAIL**

**send alert**

**check #2**

**SUCCEED**

**release resources**

**SUCCEED**

- **x_0 = 1.0**
- **v_0 = 2.0**
- **a = 4.0**
- **t_0 = 1.0**
- **t_1 = 2.0**

**compute_distance**

**assert_equal**

\[ x_t = \text{compute\_distance}(x_0, v_0, a, t_0, t_1) \]

\[ \text{call assert\_equal}(5.0, x_t) \]
Attributes of Good Unit Tests

- Silent on success
- Automated and repeatable
- Independent (no side effects)
- Transparent (obvious, but not tautological)
- Narrow/precise
- Orthogonal (1 bug ==> 1 failing test)
- Small / frugal

And in aggregate we want the tests to cover our entire application.
Test Fixtures & Parameterized Tests

- Test fixture
  - Extracts complex initialization into separate setup procedure run before test itself
  - Ensures release of resources in teardown procedure
    - Even if test fails!
  - Esp. useful if many tests share similar data structures

- Parameterized test: run multiple times but with varying inputs and expected outputs.
  - Generally used in combination with a test fixture
  - Failure messages must identify which case(s) failed
Testing Frameworks

- Greatly simplify testing
  - Test creation
    - post conditions (asserts)
    - Fixtures: set up, tear down, repeat test with different parameters
    - aggregation (test suites)
  - Test execution
    - Summary
    - Failure locations (ftest/suite name, file, line number)
    - **Informative** failure messages

- Have driven major paradigm shifts in testing methodology
  - *Developers* write tests
  - Test driven development (TDD)
The TDD Cycle

Focus on Interface

Implement Test

Focus on Algorithm

Implement Solution

Run Tests

Failure/refactor

Success

- Very small incremental changes
- What is a minimal test that moves the design forward?
- What is the smallest change to make test pass?
- Rapid cycle << 10 minutes
Perceived benefits
- High test coverage
- Software always “ready-to-ship”
- Improved productivity (and lower stress)
- Tests form a robust maintained form of documentation
- Up front focus on interfaces leads to better design.

Downside?
- 2X-3X total lines of code (tough sell to management)
- Refactoring is more difficult (but …)

Challenges
- Legacy code
- Esp. procedural legacy code

“To me, legacy code is simply code without tests.”
— Michael C. Feathers, Working Effectively with Legacy Code
Break for Questions
pFUnit

parallel Fortran Unit testing framework
pFUnit: Summary of Features

- Aimed at scientific software written in Fortran (and optionally MPI)
  - A bit of OpenMP as well (locking)
- Leverages Fortran 2003 object-oriented features
  - Very extensible
  - But … requires very recent compilers (ifort 18.03, gcc 8.2, NAG 6.2)
  - Developed with TDD
- Python base preprocessor used to simplify things that are hard/tedious in Fortran
  - Provides for expressive @ annotations (@assertEqual, @test ...)
- Various command line options: (--debug, -filter, --help, ...)
pFUnit: Assertions and Exceptions

- Vast library of numerical assertions
  - @assertEqual
    - real, complex (and integer, logical, character)
    - Kinds: default, double, REAL32, REAL64, REAL128
    - Absolute and relative tolerances (default tolerance of 0)
  - @assertLessThan, @assertGreaterThan (real)
  - Arbitrary ranks default build is max rank of 5)
    - $L_1$, $L_2$, $L_\infty$ norms for arrays (real, complex)
  - @assertIsNaN, @assertIsFinite, ...

- Exceptions implemented as a global stack (no true exceptions in Fortran)
  - Includes test name, source location, and description of failure

- Simple example: @assertEqual(3.14159, 22./7, tolerance=1.e-5)
pFUnit: Tests and Test Runners

Test declarations

- Simple `@test` annotation to indicate a subroutine is a test
- Fixture annotations:
  - `@before`, `@after`,
- Parameterized tests – advanced
  - Use by extending `ParameterizedTestCase`
  - Extension annotations: `@testCase`, `@testParameter`
- RobustRunner will attempt to run tests in a separate process
  - Can (theoretically*) handle hanging and crashing tests
  - Invoke on command line with “-r robust”
  - Alternatively run with debugging “-d”
pFUnit: MPI support

- MPI test (implemented as subclass of ParameterizedTestCase)
  - Runs a test on varying number of processes
    - Simple annotation extension – e.g., `test(npes=[1,3,7])` runs test 3 times.
    - Each instance gets new communicator with requested num. of pe's.
  - Provides simple type-bound functions to access
    - MPI Communicator (MPI_COMM_WORLD is a no-no)
    - # processes
    - MPI rank

- Exceptions and Assertions
  - Exceptions on any process gathered and reported on root process
    - Failure description decorated with process and NPES
  - Be careful: failed assertions return immediately
    - Can lead to illegal MPI calls later in test if some processes continue
    - `@mpiAssert` – Blocking; ensures all processes exit if any process fails an assertion
Examples: Installation

1. Build and install pFUnit 4.0 (develop branch)
   % git clone git://github.com/Goddard-Fortran-Ecosystem/pFUnit.git
   % cd pFUnit
   % git checkout develop
   % mkdir build
   % export PFUNIT_DIR=<prefix>
   % cmake .. -DCMAKE_INSTALL_PREFIX=$PFUNIT
   % make -j tests
   % make install

2. Clone demos repository (source)
   % git clone git://github.com/Goddard-Fortran-Ecosystem/pFUnit_demos.git
   % cd pFUnit_demos
   % ...
Example: ./Trivial

- Just the minimal amount of code, test, build/run scripts
- Elements
  - `square.F90` – the system under test
  - `test_square.pf` – a single unit test
  - `CMakeLists.txt` & `Makefile`
- Driver scripts:
  - `build_with_cmake_and_run.x`
  - `build_with_make_and_run.x`
Trivial: ./Trivial (cont’d)

```fortran
1 module Square_mod
2 contains
3 
4   pure real function square(x)
5     real, intent(in) :: x
6     square = x**2
7   end function square
8 end module Square_mod
```

Square.F90

```fortran
1 @test
2 subroutine test_square()
3   use Square_mod
4   use funit
5 
6   @assertEqual(9., square(3.), 'square(3)')
7 
8 end subroutine test_square
```
test_square.pf
Example: ./Trivial (cont’d)

```bash
1  cmake_minimum_required(VERSION 3.12)
2  
3  project (PFUNIT_DEMO_TRIVIAL
4      VERSION 1.0.0
5      LANGUAGES Fortran)
6  
7  find_package(PFUNIT REQUIRED)
8  enable_testing()
9  
10  # system under test
11  add_library (sut
12      square,F90
13  )
14  target_include_directories(sut PUBLIC ${CMAKE_CURRENT_BINARY_DIR})
15  
16  # tests
17  set (test_srcs test_square.pf)
18  add_pfunit_c test (my_tests
19    TEST_SOURCES ${test_srcs}
20    LINK_LIBRARIES sut
21  )
```

CMakeLists.txt

Include pFUnit

Macro to build test
Example: ./Trivial (output)

One “.” per test - to monitor progress

Time: 0.000 seconds
OK
(1 test)
Example: ./Basic

Demonstrates a variety of basic pFUnit features and capabilities

- Source directory has 2 implementations: working and broken
  - Implement elemental square() function and integer factorial function
- Basic assertions: test_simple.pf
- See what failure messages look like: test_failing.pf
- Various mechanisms to skip tests: test_disable.pf
  1. @disable annotation – test not run, but tallied in summary
  2. !@test not mentioned at all
  3. @test(#ifdef=foo) – test is run if -Dfoo
  4. @test(#ifndef=foo) – test is run if not -Dfoo
- Very simple example using setup and teardown methods: test_simple_fixture.pf
- Testing source code error handling: test_error_handling.pf
`bash-3.2$ ./broken_tests`  

```
.F.F.F
```

Time: 0.001 seconds

Failure

in:
test_failing_suite.test_assert_true_and_false_fail

Location:
[test_failing.pf:14]

intentionally failing test

...
Failure in:
\texttt{test\_failing\_suite.test\_assert\_equal\_fail}

\textbf{Location:} \[\texttt{test\_failing.pf:26}\]

intentionally failing test

\textbf{AssertEqual failure:}
- \textit{Expected:} \(<9.000000>\)
- \textit{Actual:} \(<9.000988>\)
- \textit{Difference:} \(<0.9880066E-03>\) (greater than tolerance of \(0.1000000E-03\))

Failure in:
\texttt{test\_failing\_suite.test\_fail\_array}

\textbf{Location:} \[\texttt{test\_failing.pf:36}\]

intentionally failing test

\textbf{ArrayAssertEqual failure:}
- \textit{Expected:} \(<4.000000>\)
- \textit{Actual:} \(<4.410326>\)
- \textit{Difference:} \(<0.4103265>\) (greater than tolerance of \(0.1000000\))
  at index: \([2]\)
FAILURES!!!
Tests run: 3, Failures: 3, Errors: 0
, Disabled: 0
ERROR STOP: *** Encountered 1 or more failures/errors during testing. ***
pFUnit: disabled test output

bash-3.2$ ./disabled_test
.I..
Time: 0.000 seconds

OK
(3 tests, 1 disabled)
pFUnit: disabled test output

bash-3.2$ ./disabled_test -d

Start: <test_disable_suite.test_1_active>
  .   end: <test_disable_suite.test_1_active>

Disable: <test_disable_suite.test_2_disabled>
I

Start: <test_disable_suite.test_3_active>
  .   end: <test_disable_suite.test_3_active>

Start: <test_disable_suite.test_if_not_foo_defined>
  .   end: <test_disable_suite.test_if_not_foo_defined>

Time: 0.001 seconds

OK
(3 tests, 1 disabled)
Demonstrates tests for MPI-based software:

- **Tests:** test_halo.pf
- **Build:** CMakeLists.txt
- **Things we want to test**
  1. Rank of neighbors
  2. Interior not changed
  3. Halo filled from neighbor values

---

**Example: ./MPI**

- 2D arrays with 1D domain decomposition
- **Not** periodic

Halo/guard cells on North

Halo/guard cells on South
Example: ./MPI (cont’d)

```fortran
  @test(npes=[1,2,3,4])

  subroutine test_fill_halo_interior(this)
      type (MpiTestMethod), intent(inout) :: this
      real :: array(NX_LOC,0:NY_LOC+1) ! local domain with halo region
      real :: interior_value

      ! Preconditions: Initialize interior and halos
      interior_value = this%getProcessRank()
      array(1:NX_LOC,1:NY_LOC) = interior_value
      array(1:NX_LOC,0) = HALO_UNDEF
      array(1:NX_LOC,NY_LOC + 1) = HALO_UNDEF

      ! Invoke SUT
      call fill_halo(array, this%getMpiCommunicator())

      ! check that interior values are unchanged
      @MPIassertEqual(interior_value, array(1:NX_LOC,1:NY_LOC))

  end subroutine test_fill_halo_interior
```
Example: ./MPI (cont’d)

```fortran
subroutine test_fill_halo_south_pole(this)
  type (MpiTestMethod) :: this

  integer :: rank
  real :: array(NX_LOC,0:NY_LOC+1)
  real, parameter :: INTERIOR_VALUE = 1.

  ! Preconditions
  array(1:NX_LOC,0) = HALO_UNDEF
  array(1:NX_LOC,NY_LOC + 1) = HALO_UNDEF
  array(1:NX_LOC,1:NY_LOC) = INTERIOR_VALUE

  call fill_halo(array, this%getMpiCommunicator())

  rank = this%getProcessRank()
  if (rank == 0) then  ! southern halo
    @assertEqual(HALO_UNDEF, array(1:NX_LOC,0))
  end if
end subroutine test_fill_halo_south_pole
```
Example: ./MPI (cont’d)

```fortran
100  @test(npes=[1,2,3])
101  subroutine test_fill_halo_south_other(this)
102      type (MpiTestMethod) :: this
103
104      integer :: rank
105      real :: array(NX_LOC,0:NY_LOC+1)
106
107      ! Preconditions
108      array(1:NX_LOC,0) = HALO_UNDEF
109      array(1:NX_LOC,NY_LOC + 1) = HALO_UNDEF
110      array(1:NX_LOC,1:NY_LOC) = rank
111
112      call fill_halo(array, this%getMpiCommunicator())
113
114      rank = this%getProcessRank()
115      if (rank > 0) then ! southern halo
116          @assertEqual(rank - 1, array(1:NX_LOC,0))
117      end if
118
119   end subroutine test_fill_halo_south_other
```
Examples: ./MPI output

test 1
  Start 1: mpi_tests

1: Test command: /Users/tclune/installed/Compiler/nag-6.2_clang-
  9.1/openmpi/3.1.2/bin/mpirun "--oversubscribe" "-np" "4" "mpi_tests"
1: Test timeout computed to be: 10000000
1: ..................
1: Time:         0.001 seconds
1: OK
1: (18 tests)
1: 1/1 Test #1: mpi_tests ......................... Passed   0.13 sec

100% tests passed, 0 tests failed out of 1

Total Test time (real) =   0.14 sec
What is new in pFUnit 4.0 (beta)

- Major cleanup of source code and build system
  - Single build for serial and MPI (and ESMF tests)
  - Very few compiler warnings, compiler #ifdef’s …
- (Possibly) improved RobustRunner – for crashes and hangs
- Extensible annotations: @disable, @timeout(0.5), …
  - Users can add their own (funitproc needs some tweaks)
- Miscellaneous
  - Improved build macros (cmake and make) for creating executable tests
  - Support for Test Anything Protocol (TAP)
  - Support for testing Earth System Modeling Framework (ESMF) gridded components
fHamcrest (Fortran version of hamcrest)

- **Composable** system of "matchers" – leads to significantly improved extensibility
- **Self-describing** – better error messages
- Assertions *read almost like sentences*
- Simple examples:

```plaintext
@assert_that(x, is(equal_to(5))
@assert_that([i,j,k], is_not(permutation_of([1,2,3]))
@assert_that(x, is(all_of([greater_than(0),less_than(5)]))
```

- What about MPI?
  - Not in 4.0 due to a technical issue that needs to be resolved
  - But expect it to look something like:

```plaintext
@assert_that(x, on_process(5, comm, is(relatively_near(10.,0.1))))
@assert_that(x, on_all_processes(comm, is(equal_to(5))))
```
Summary

- **pFUnit 4.0 (beta)** has been released as 4/7/2019
  - Please try it out!

- Expected in 4.1
  - Coarray based tests with CAF_TestCase
    - Requires F2018 teams to be useful
  - Extending fHamcrest
    - Esp. pfHamcrest
References

- Junit: https://github.com/junit-team
- pFUnit: https://github.com/Goddard-Fortran-Ecosystem/pFUnit
- Test-Driven Development: By Example, Kent Beck
- Working Effectively with Legacy Code, Michael Feathers
Questions?

(Stick around for discussion about testing obstacles and mitigations.)
Testing challenges, misconceptions, and methodologies

- Many issues can complicate and even appear to prevent useful unit testing
  - Complexity
  - Floating-point (inexact) arithmetic
  - Distributed parallelism
  - Scalability – testing at petascale, exascale, and beyond

- Many/most of these can be addressed or mitigate by 2 complementary techniques:
  - Use very fine-grained units (subroutines, functions)
  - Use software “mocks” to sidestep complex dependencies.
  - What are mocks? Since you asked …
Software Mocks

Mock provides same interface but can be configured to verify inputs and produce preprogrammed outputs.
Mock Example: Coupled Climate

**AOGCM**

Test?

**AGCM**

Impossible to specify initial conditions with simple obvious outputs

**OGCM**

**Mock AGCM**

Mock AGCM provides wind stress and expect surface Temp

**Mock AOGCM**

**Mock OGCM**

Mock OGCM provides surface temp and expects wind stress
Challenge: Algorithmic Complexity

- Irreducible complexity?
  - E.g., test of climate model is as complex as climate model?
  - No - each software component is tested in isolation. Complexity is $O(N)$.
  - Essential approach: software “mocks” for nontrivial dependencies

- Lack of analytic solutions?
  - Partial confusion of verification and validation
  - Problem is actually that the SUT is too large.
  - Mitigation
    - Split calculation into small units
    - Lowest levels are easily tested in isolation
    - Higher levels are tested with mocks (still coming back to that)
  - Mitigation of the mitigation – 2 implementations: fused and fine-grained
Challenge: Inexact arithmetic

- Assertions for FP results must generally specify a tolerance
- Estimating a reasonable tolerance is *problematic*
  - Too tight – correct implementation fails
  - Too loose – incorrect implementation succeeds
  - Even when good bounds estimate is available it is impractical
    - E.g. RK4 has error that is $O(h^5)$, but what is the leading coefficient?
    - And who has spare applied mathematicians lying around?
  - Temptation: increase tolerance until test passes (assumes SUT is already correct)
Challenge: Inexact arithmetic (cont’d)

- What gives rise to (nontrivial) roundoff?
  - Subtraction of nearly equal values
  - Iterated operations
  - ...

- Mitigation 1: Use smart input values such that arithmetic is nearly exact
  - You don’t need to use physically realistic values to test an expression.
  - Trivial example on next slide.

- Mitigation 2: Split complex expressions into nested pieces.
  - Test pieces separately with near-exact arithmetic

- Mitigation 3: Split test of iterated calculation
  1. Test individual iteration with smart input values
  2. Test that iteration iterates
Consider a test for a procedure that calculates the area of a circle:
```fortran
@assertEqual(3.14159265, area(r=1.))
@assertEqual(12.56637060, area(r=2.))  ! Is this output obvious?
```

Instead we create a helper function that takes pi as a parameter.
```fortran
  real function area_internal(pi, r)
    area_internal = pi*r**2
  end function

  real function area(r)
    use math_constants, only: pi
    area = area_internal(pi, r)
  end real function
```

Now we can test in a sensible manner:
```fortran
@assertEqual(3, area_internal(pi=3., r=1.))
@assertEqual(12, area_internal(pi=3., r=2.))
@assertEqual(area_internal(pi=pi,r=2.), area(r=2.))
```
Challenge: Distributed parallelism

- Trivial issues: exercising on multiple processes, collecting exceptions, …
  - pFUnit – been there, done that.
- Real challenges: tests of functionality that may rely on timing
  - Race condition, deadlock, livelock, …
- Solution: Mock MPI (analog of “brain in a vat”)
  - Serial software layer with same interfaces as MPI
  - Externally configurable to control MPI outputs
  - Single process of application “sees” a parallel env.
- Example: Testing mutex
  - Cases:
    - I request mutex, and no one else has it
    - I request mutex, but someone else has it
    - I release mutex, but must notify other waiter
    - I release mutex, and there is no other waiter
Challenge: Exascale

- Some defects are only apparent at extreme scale
  - Large number of processes
  - Large memory
- Debugging at extreme scale is expensive
  - Consumes expensive computing resources
  - Developer idle – waiting for queue
  - Delivery is delayed
- Once fixed, how do we ensure fix is preserved?
  - Routine testing too expensive

- Approach: use Mock MPI
  - Use Mock MPI to simulate the exascale environment experienced by a process or node.
  - Replicate issues on a workstation
  - Run "exascale" regression tests on demand.
Thank you!

(Questions)