Testing Scientifc Software: Challenges and Remedies

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Outline

- Overview of unit testing and testing frameworks
- Simple examples with pFUnit – a testing framework for Fortran + MPI
- Scientific/numerical software: obstacles and remedies

Scientific Software Development

Objective Reality

Theory and Data

Mathematical Model

Discretization & Approximation

Implementation

Executable

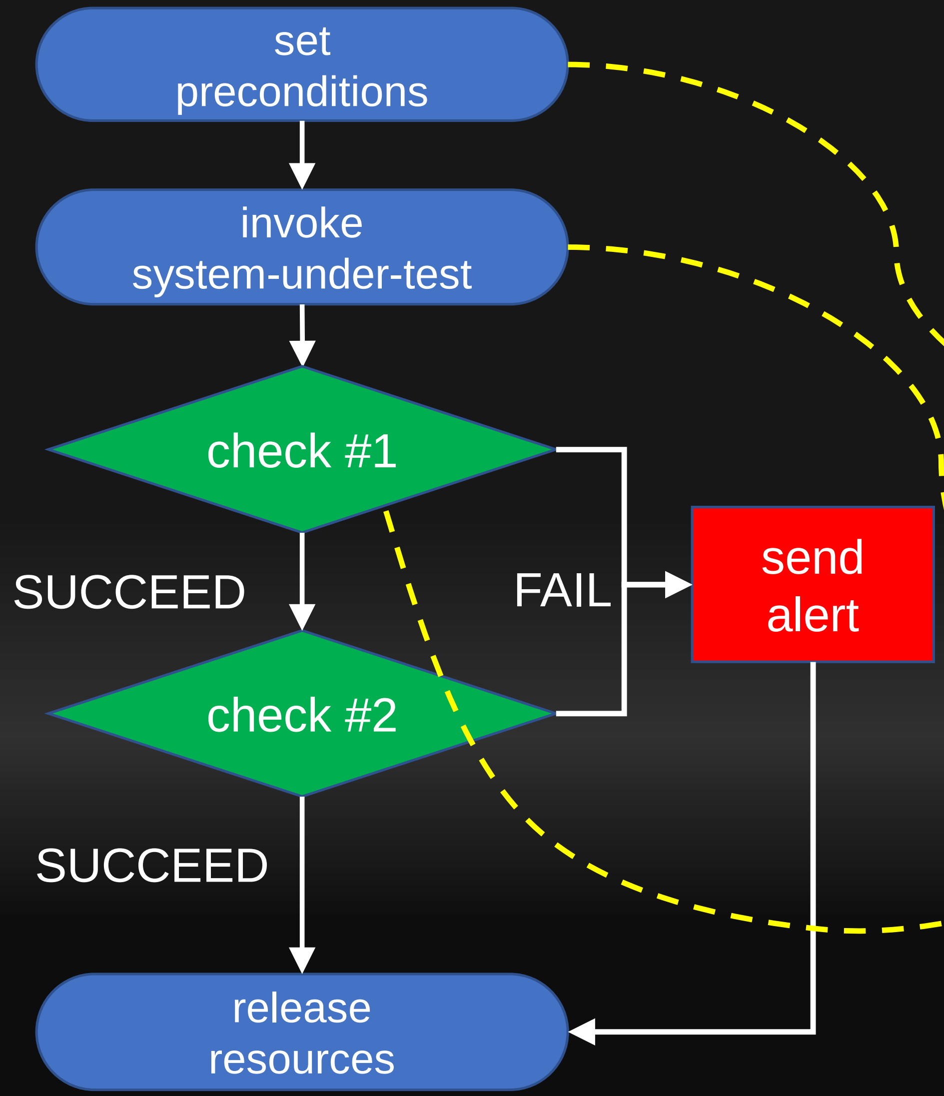
output

Software Verification

Validation: Does the SW produce desirable results? E.g., how accurate is this weather forecast?

Verification: Does the SW correctly implement our model? Do changes preserve behavior? E.g., strong reproducibility, checkpoint-restart, …

Anatomy of a Unit Test



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

```
x0 = 1.0
v0 = 2.0
 a = 4.0
t0 = 1.0
t1 = 2.0
```

```
x_t = compute_distance(x0, v0, a, t0, t1)
```

```
call assert_equal(5.0, x_t)
```

Attributes of Good Unit Tests

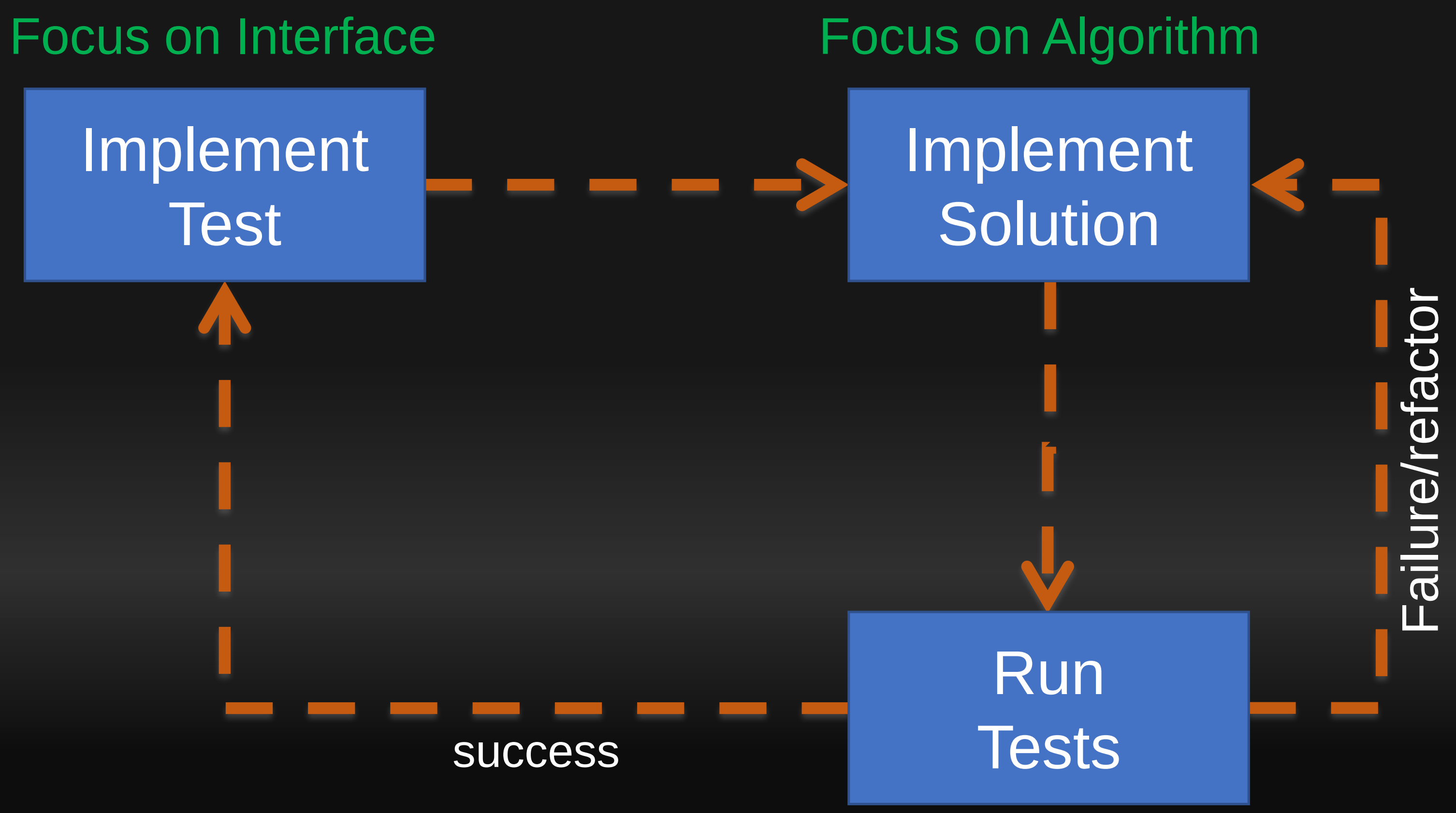
- ✓ Silent on success
- ✓ Automated and repeatable
- ✓ Independent (no side effects)
- ✓ Transparent (obvious, but not tautological)
- ✓ Narrow/precise
- ✓ Orthogonal (1 bug ==> 1 failing test)
- ✓ Small / frugal

And in aggregate we want the tests to cover our entire application.

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



- 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

TDD

- 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

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_∞ 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 Asssertions
  - 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

pFUnit Installation and Examples

1. Build and install pFUnit 4.0 (develop branch)

```
% git clone git://github.com/Goddard-Fortran-Ecosystem/pFUnit.git
% cd pFUnit
% 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)

```
module Square_mod
contains

   pure real function square(x)
      real, intent(in) :: x
      square = x**2
   end function square
end module Square_mod

```

Square.F90

test_square.pf

```
@test
subroutine test_square()
   use Square_mod
   use funit

   @assertEqual(9., square(3.), 'square(3)')

end subroutine test_square
```

Other simple examples

```
@assertEqual(6, factorial(3))
@assertEqual(1, factorial(1))
@assertEqual(1, factorial(0))

y = solve(f, b, tol)
@assertLessThanOrEqual(abs(f(y)-b), tol) ! Tolerance in y
@assertLessThanOrEqual((f(x+tol)-b)*(f(x-tol)-b), tol) ! Tolerance in x
```

pFUnit: output from failing tests (1 of 3)

```
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
  …
```

progress bar – 3 tests; 3 failed

Extra message supplied by developer

pFUnit: output from failing tests (2 of 3)

```
…
Failure
 in:
test_failing_suite.test_assert_equal_fail
  Location:
[test_failing.pf:26]
intentionally failing test
AssertEqual failure:
      Expected: <9.000000>
        Actual: <9.000988>
    Difference: <0.9880066E-03> (greater than tolerance of 0.1000000E-03)

Failure
 in:
test_failing_suite.test_fail_array
  Location:
[test_failing.pf:36]
intentionally failing test
ArrayAssertEqual failure:
      Expected: <4.000000>
        Actual: <4.410326>
    Difference: <0.4103265> (greater than tolerance of 0.1000000)
      at index: [2]
```

<suite_name>.<test_name>

[<file>:<line_number>]

Failure description

Index of first incorrect element

pFUnit: failing test output (3 of 3)

```
…
 FAILURES!!!
Tests run: 3, Failures: 3, Errors: 0
, Disabled: 0
ERROR STOP: *** Encountered 1 or more failures/errors during testing. ***
```

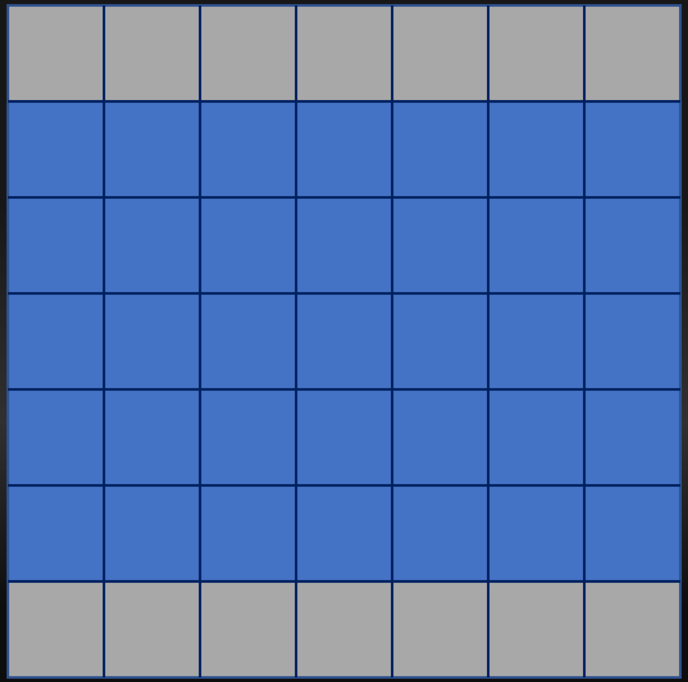
summary

Example: ./MPI

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

Halo/guard cells on North



Halo/guard cells on South

2D arrays with
1D domain decomposition
Not periodic

Example: ./MPI (cont’d)

```
@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)

```
   @test(npes=[1,2,3])
   subroutine test_fill_halo_south_other(this)
      type (MpiTestMethod) :: this

      integer :: rank
      real :: array(NX_LOC,0:NY_LOC+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) = rank

      call fill_halo(array, this%getMpiCommunicator())

      rank = this%getProcessRank()
      if (rank > 0) then ! southern halo
         @assertEqual(rank - 1, array(1:NX_LOC,0))
      end if

   end subroutine test_fill_halo_south_other
```

What is new in pFUnit 4.0

- 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

New in 4.0 (cont'd)

- 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:

```
@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:

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

Challenges For Scientific Software?

- Legacy code (esp. procedural legacy code)
- Complexity?
- Inexact floating-point arithmetic
- Lack of analytic test cases?
- Parallelism
- Extreme scalability

- General techniques for addressing/mitigating?
  - Intelligent selection of preconditions
  - Write software (and tests) at a very fine-grained level
  - Replace complex dependencies with “mocks” (defined in a few slides)

Challenge: Floating-point arithmetic

- Inexact → test assertions require us to specify a *tolerance*
  - Too loose – incorrect implementation passes test
  - Too tight – correct implementation fails test

- How do we determine an appropriate tolerance?
  - *Avoid the temptation to just increase tolerance until test passes (assumes SUT is correct)*
- Observation: FP arithmetic is **exact** for some values:
  - Addition, subtraction, multiplication, exponentiation of small integer values
  - Division is somewhat trickier, but still many exact combinations
- Strategy:
  - Break complex expressions into sub-expressions that are easily tested with ”exact” arithmetic
  - Remember: test your code, not the compiler nor the math library.

Example: Testing FP expressions

How would we test a procedure that should compute: y(x) = (A + B x + C x^2) / (E x + 1)

Step 1: Split into 3 helper functions with extra parameters

y1(x; a,b,c) = a + b x + c x ^2

y2(x; e) = e x + 1

y3(n, d) = n/d

Step 2: Now implement y(x) as y(x) = y3(y1(x; A,B,C), y2(x; E))

Step 3: Test each piece with simple values

y1(2.; 3.,1.,2.) == 13.?

y2(3.; 2.) == 7.?

Q1: Should we test y3?

Q2: Should we test y directly?

Roundoff that grows?

- Iteration can result in roundoff-errors that grow quickly
  - Indeed – this is true of other sources of error: consider Forward Euler time integration

- Mitigation:

1. Implement and test isolated iteration as separate procedure
   - As before, use synthetic inputs to sidestep tolerance issue
2. Separately test the loop *logic*
   - # of iterations
   - Exit criteria
   - …

- But what about performance …?

Challenge: Lack of Analytic Constraints

- Mitigation
  - Split implementation into smaller pieces
  - Test lowest level “leaf” procedures directly
  - Test higher level procedures by mocking lower levels (still coming to the definition of “mock”)

- Problem: fine-grained implementation may be slower

- Mitigation of the mitigation – maintain 2 implementations
  - Fine-grained implementation tested directly as outlined above
  - Fused implementation is tested against fine-grained implementation
  - Note: the tolerance question now returns.
    - Often machine epsilon is good enough at -O0
    - Really just want to ensure that the fusion was performed correctly

Warmup: Runge-Kutta 4^{th} Order

$$y_{n+1} = y_n + 1/6(k_1 + 2k_2 + 2k_3 + k_4)$$
$$k_1 = h\, f(y_n)$$
$$k_2 = h\, f(y_n + k_1/2)$$
$$k_3 = h\, f(y_n + k_2/2)$$
$$k_4 = h\, f(y_n + k_3)$$

Problem: How to implement nontrivial, nontautological test?

Subsequent sub steps are nontrivial function of inputs

Solution: Choose a non-realistic nontrivial test function F(y) that ***ignores*** its argument

F(y) = 2 ! 1st invocation

F(y) = 1 ! 2nd invocation

F(y) = 3 ! 3rd invocation

F(y) = 2 ! 4th invocation

Tests:

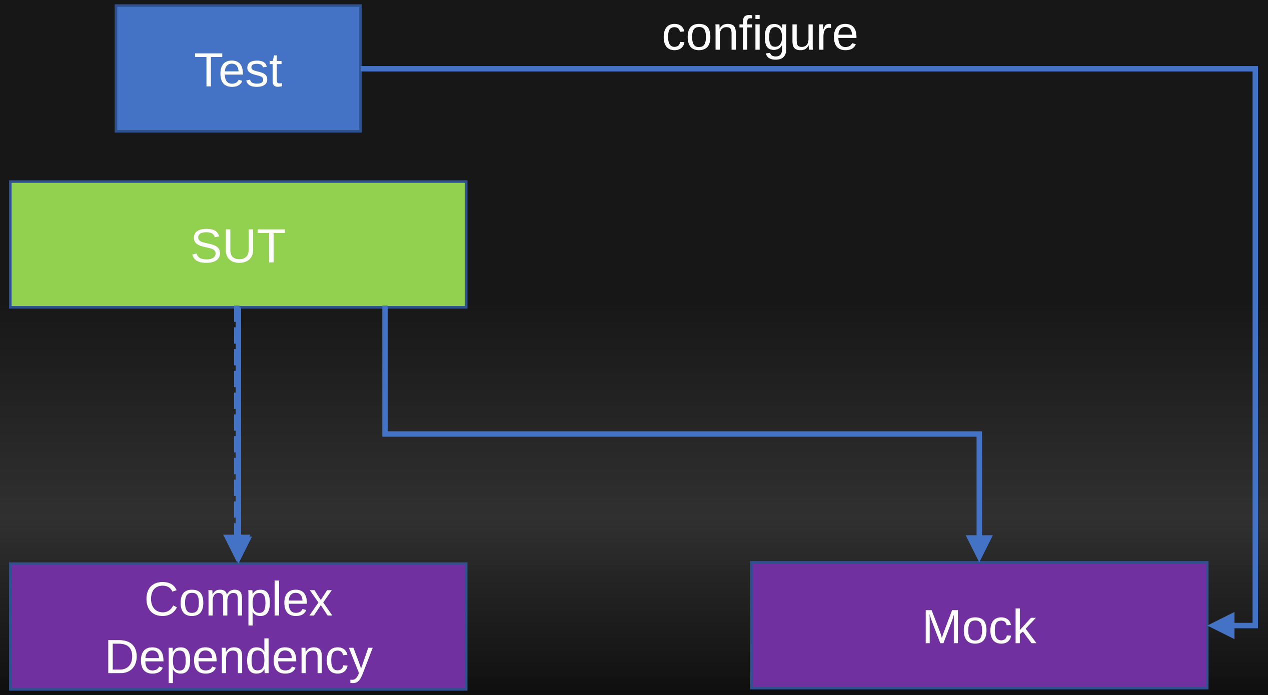
$y_{n+1}(h=1) == y_n + 2$

$y_{n+1}(h=2) == y_n + 4$

Other tests?

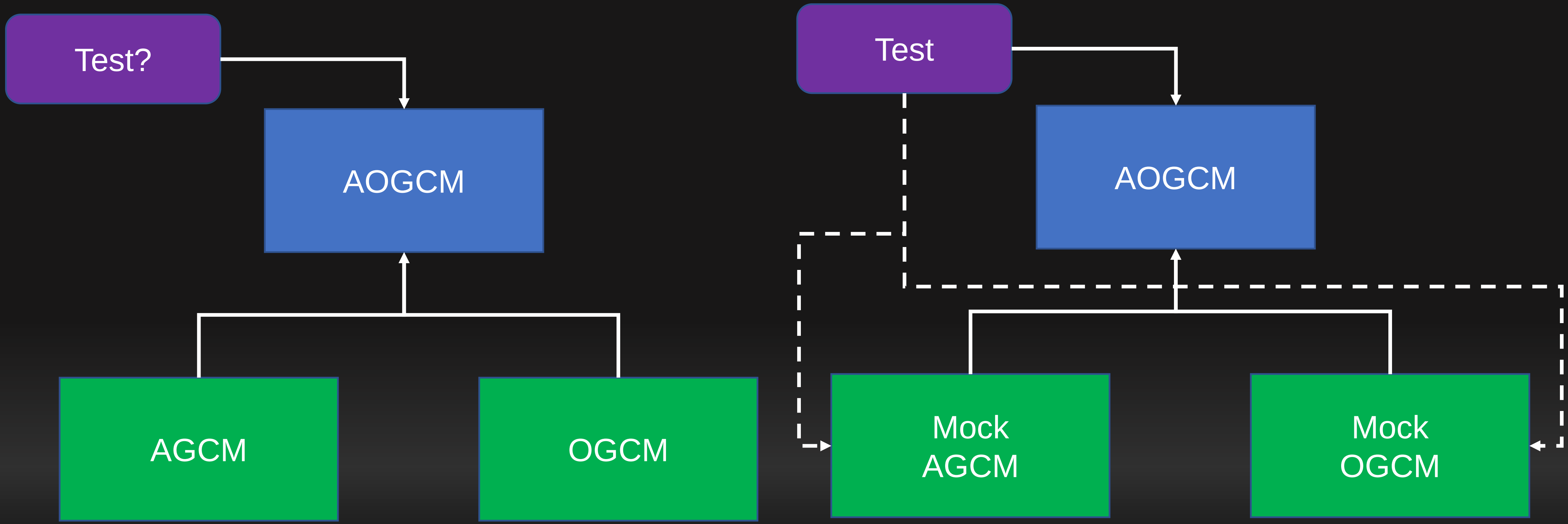
- Is 1st argument to F is y_n?
- Is 2nd argument to F is $y_n + 2/2$?
- Etc.

Software Mocks



Mock provides same interface but can be configured to verify inputs and produce preprogrammed outputs

Mock Example: Coupled Climate



Impossible to specify initial conditions with simple obvious outputs

Mock AGCM provides wind stress and expect surface Temp

Mock OGCM provides surface temp and expects wind stress

Challenge: Distributed parallelism

- Trivial issues: exercising on multiple processes, collecting exceptions, …
  - pFUnit – been there, done that.
- Real challenges: tests of logic that depends on timing
  - Race condition, deadlock, livelock, …
  - E.g., how would you test the implementation of a barrier?
    - Dangerously similar to the Halting Problem

- Approach: 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
  - NOT the same thing as an MPI stub layer!
  - Originally suggested to by Hal Finkel (ANL) in exascale context

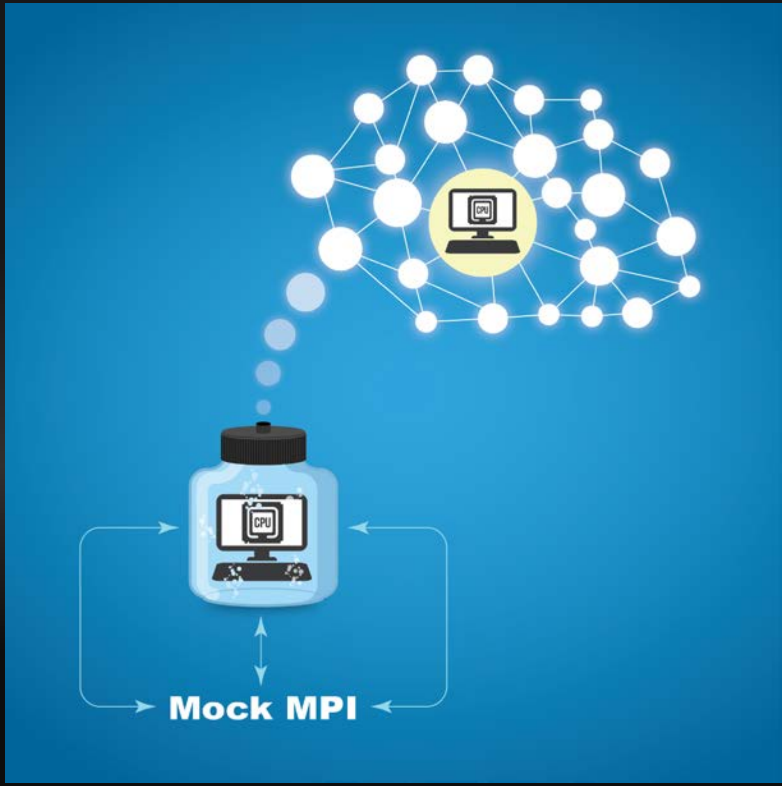


Image: Sterling Spanger NASA/GMAO

Example Testing Mutex Implementation

- MPI provides low-level locking mechanism, but not a true mutex
- Proper implementation of mutex using low-level mechanism is nontrivial
- Need to test several cases:
  - P request mutex, and no other process has it
  - P requests mutex, but Q has it; P should receive notification from Q (test for recv)
  - P releases mutex, no other process waiting;
  - P releases mutex, Q is waiting;   P should notify Q (test for send)
- Could possibly use manual delays to arrange each possibility
  - Messy, error prone, and some combinations lead to deadlock in the test itself
- Mock of MPI makes these tests straightforward
  - Weird consequence: tests are ***serial*** applications

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

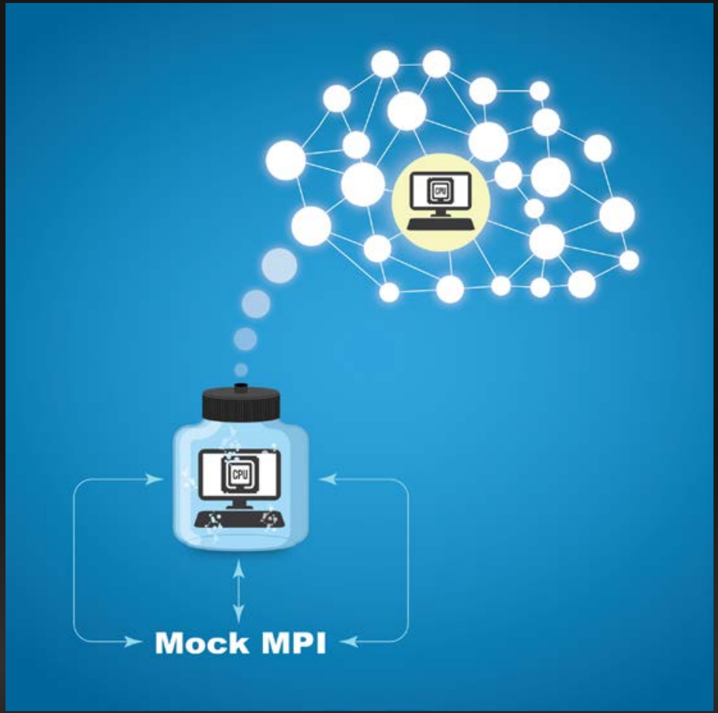


Image: Sterling Spanger NASA/GMAO

- 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.

Summary

- Unit testing of scientific software has become mainstream.
- Techniques to address/mitigate testing of unique aspects of scientific software exist.
- The hard question: Is the extra effort worth it?

- pFUnit 4 has been released as 5/5/2019 – please try it out!

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
- T. Clune, H. Finkel, and M. Rilee "Testing and Debugging Exascale Applications by Mocking MPI", SE-HPCCSE, 2015.
- T. Clune and R. Rood, "Software Testing and Verification in Climate Model Development", IEEE Software Volume 28 Issue 6, November 2011.

Thank you!

(Questions)

Not all tests are created equal

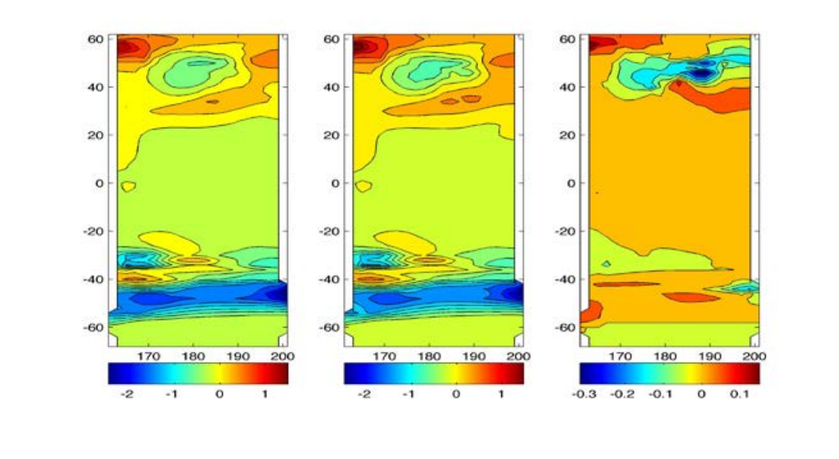
- Abort?:

```
if (x < 0.0) ERROR STOP "ILLEGAL VALUE FOR X"
```

- Diagnostic print statement:

```
print*, "loss of mass = ", deltaMass
```

- Visual inspection / acceptance threshold for regression:



Test Fixtures & Parameterized Tests

- Test fixture
  - Extracts complex/expensive 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 preconditions (inputs)
  - Generally used in combination with a test fixture
  - Failure messages must identify which case(s) failed

Example: ./Trivial (cont'd)

```
cmake_minimum_required(VERSION 3.12)

project (PFUNIT_DEMO_TRIVIAL
  VERSION 1.0.0
  LANGUAGES Fortran)

find_package(PFUNIT REQUIRED)
enable_testing()

# system under test
add_library (sut
  square.F90
  )
target_include_directories(sut PUBLIC ${CMAKE_CURRENT_BINARY_DIR})

# tests
set (test_srcs test_square.pf)
add_pfunit_ctest (my_tests
  TEST_SOURCES ${test_srcs}
  LINK_LIBRARIES sut
  )
```

CMakeLists.txt

Include pFUnit

Macro to build test

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)
```

debug option

Start/end progress

disabled in summary

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:
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
```

Each #pes is different test

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 mitigated by 2 complementary techniques:
  - Use very fine-grained units (subroutines, functions)
  - Use software “mocks” to sidestep complex dependencies.
  - What are mocks? Since you asked …

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

Example: The Indiana Pi Bill (this really happened)

- Consider a test for a procedure that calculates the area of a circle:

```
@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.

```
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:

```
@assertEqual(3, area_internal(pi=3., r=1.))
@assertEqua (12, area_internal(pi=3., r=2.)
@assertEqual(area_internal(pi=pi,r=2.), area(r=2.))
```

Example: ./Trivial (output)

One "." per test - to monitor progress

```
.
Time:              0.000 seconds

OK
(1 test)
```

Success/status

Example: ./MPI (cont'd)

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